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MODELLING OF FUNCTIONAL PROPERTIES OF SHAPE MEMORY ALLOY BY MACHINE LEARNING METHODS

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Abstract. *This study deals with the modelling of NiTi shape memory alloy dissipated energy by means of supervised machine learning methods, considering the loading frequency. Shape memory alloys are materials of high interest both to science and industry. These materials are enjoying wide popularity due to their two peculiar properties: unique effect of shape memory and superplasticity, caused by direct austenite-martensite phase transformation and reverse martensite-austenite transformation. The traditional deterministic methods of assessment of material properties are often costly, time-consuming, and demand a well-trained workforce and laboratory equipment. On the contrary, in recent years, the methods of artificial intelligence have gained widespread attention due to their ability to reveal hidden insights from existing data. Machine learning is a subset of artificial intelligence. It allows training based on the available data and becomes better with time without the explicit need to be programmed. The experimental dataset was taken from open scientific sources. It contained the hysteresis curves for six loading frequencies of 0.1, 0.5, 1, 5, 7, and 10 Hz. The input data consisted of the next features: stress s (MPa), cycle number N, and loading frequency f (Hz). Based on these data, for each loading cycle, and for each loading cycle, the dissipated energy was calculated. To remove noise, Locally Weighted Scatterplot Smoothing (LOWESS) smoother in the nonparametric package of statsmodels was utilized. After that, the trapezoid numerical integration method was employed to calculate the area enclosed by the hysteresis loop of the respective cycle, that is, the dissipated energy. To augment the dataset, its points were interpolated using the modified Akima interpolation method (makima). Four models were built using the methods of Random Forest, AdaBoost, Gradient Boosting, and Neural Network. The best results were shown by the ensemble methods, such as AdaBoost, and Random Forest. For instance, the MAPE of AdaBoost was just 0.074, whereas the MAPE of Random Forest was 0.144. It was found that the Gradient Boosting method and Neural Network are not suitable for such a dataset, since the errors are quite large and, therefore, these methods are not good enough to be employed for solving such a problem.*

Key words: *shape memory alloy, machine learning, dissipated energy, random forest, AdaBoost, decision trees, data science, data analytics; data mining, big data, regression problem.*

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1. INTRODUCTION

Traditional, so-called classical materials, such as various metals and alloys, played a key role as the structural elements for quite a long time [1]. Engineers of the past designed the devices and chose the alloys by employing the classical engineering approach to comprehend the macroscopic properties of the materials and select the appropriate ones that allowed them to provide the required functionality for certain applications [2]. With the advances in material science as well as with the increase in structure size and logistic limitations, scientists have continuously invented new high-quality materials for numerous practical needs [2]. The eternal and unchanged aim of the engineers in most cases is the improvement of structures' efficiency and decreasing their weight without loss of costs or technical properties. To achieve this goal, the change of multicomponent systems for a smaller number of lightweight, highly productive components is quite promising [2, 3]. Such modern materials played a dominant role in the development of numerous engineering innovations and achievements, such as Airbus A380, Boeing 787 Dreamliner, reliable cars

with low consumption of fuel, better methods of drug delivery, etc [4]. Ingenious commercial products in various areas of engineering science correspond to all the requirements, due to the advancements of numerous latest technologies and satisfying the challenges of tomorrow's needs [4].

Shape memory alloys (SMAs) are materials of high interest both to science and industry [5]. These materials are enjoying wide attention due to their two peculiar properties: unique effect of shape memory and superplasticity, caused by direct austenite-martensite phase transformation and reverse martensite-austenite transformation [6, 7]. A lot of types of SMAs are already known, for instance, the most ubiquitous are alloys based on Ni, Fe, Cu, and magnetic SMAs [1]. One of the examples of magnetic SMA is Ni-Mn-Ga.

The examples of commercially available SMAs are alloys based on Co-Al-Ni, Fe-Mn-Si, Co-Zn-Al, and Ni-Ti, the latter of which is the most widespread due to its best replication thermomechanical characteristics, the higher strength, big hysteresis loops, and biocompatibility [8, 9]. Also, the two-component (binary) NiTi SMA is the material that is most widely used among the already known SMAs, since it can recover after the strains that reach up to 8% [10]. The binary NiTi shows not only one-way SMA, but also the superplasticity and two-way shape memory effect, which can be altered by changing the amount of Ni in the alloy and using the thermomechanical treatment [11].

SMAs can recover their initial shape by memorising it between two transformation phases, which depend on external factors, such as temperature, loading, or magnetic field. There are two known phases of SMA: parent phase (austenite), which is stable under high temperatures, and the derived phase (martensite), which is stable at low temperatures. Due to its relative softness, SMA is easily deformed in the martensite phase. Austenite phase is a well-formed body-centered cubic structure with one variant. Martensite phase is characterized by low symmetry, and, depending on phase transition, can exist in various configurations (monoclinic, orthorhombic, and rhombohedral structures) [12].

The classical deterministic methods of assessment of the material properties are often costly and time-consuming, and require a well-trained workforce and laboratory equipment. On the contrary, in recent years, the methods of artificial intelligence (AI) have gained widespread attention due to their abilities to reveal hidden insights from a large amount of existing data of various natures. Machine learning (ML) is a subset of AI. It allows training based on the available data and becomes better with time without the explicit need to be programmed. Methods of ML allow us to find dependencies that exist in the available datasets, and based on them, perform the predictions or take certain decisions [13].

In recent decades, ML has become one of the main trends and cutting-edge information technologies, and a basic and integral attribute of everyday life. The amount of information is being increased exponentially, and there emerges the requirement to analyse it to get the hidden and non-obvious dependencies among the data [13].

ML has found its application in various fields of science and technology. It is the number of algorithms that allow us to understand data and their nature [14]. In general, these algorithms can be divided into the following: supervised learning and unsupervised learning. Overall, methods of ML are based on the construction of a statistical model for the prediction or estimation of the target based on at least one input variable, also known as a feature. Such problems often emerge in business, medicine, finance, psychology, engineering, and other areas of human activity. On the contrary, unsupervised learning utilizes the input variables, or features, but the target is not given. In this case, it is possible to study the dependencies and structure of the data of such nature.

Therefore, due to SMAs unique properties and their practical use in science and technology, it is of high importance to investigate the functional and structural properties of SMAs, considering the effect of loading frequency.

There are quite a lot of studies that deal with the SMAs, modelling of their functional and structural properties of SMA using various methods of ML [15–18].

However, as far as the authors knowledge goes, the study of the loading frequency effect on the dissipated energy of NiTi SMA by means of supervised ML methods remains unaddressed.

This work focuses on the investigation of the effect of test loading frequency on the functional properties, namely, on the dissipated energy of loading cycle based on various supervised learning methods.

2. EXPERIMENTAL METHODS

The experimental dataset was taken from the study [19]. It contained the hysteresis curves for six loading frequencies of 0.1, 0.5, 1, 5, 7 and 10. The input data consisted of the next features: stress □ (MPa), cycle number N, and loading frequency f (Hz). Based on these data, for each test frequency, and for each loading cycle, the dissipated energy was calculated using the following procedure. At first, each loading cycle was divided into loading and unloading part. Since the experimental data are often noisy, an additional smoothing was employed. The preprocessing script was written in Python 3.10 programming language. Namely, to remove the noise in experimental data, Locally Weighted Scatterplot Smoothing (LOWESS) smoother in the nonparametric package of statsmodels was utilized [20]. LOWESS performs weighted local linear fits. LOWESS is a non-parametric regression method used to create a smooth line or curve through a scatterplot of data. It visually represents the general trends and patterns in a dataset without making strong assumptions about the data underlying structure. The locally weighted means that a regression is performed on small subsets of the data, with points closer to the central point of that subset receiving more weight in the calculation of the smoothed value.

Instead of fitting a single line or curve to the entire dataset, LOWESS fits a series of regression models to small, localized portions of the data. For each point on the resulting smooth curve, a regression is performed using the surrounding data points. Points closer to the point being smoothed are given higher weights than those further away. The weighted regressions are combined to create a smooth, flexible curve that passes through the data, revealing underlying trends and minimizing noise. LOWESS can be made more resistant to outliers by using a robust weighting function, which further downweights extreme data points that might distort the trend.

After that, the trapezoid numerical integration method was employed to calculate the area enclosed by the hysteresis loop of the respective cycle, that is, the dissipated energy W_{dis}.

Afterwards, to augment the dataset, the points of the dataset were interpolated using the modified Akima interpolation method (makima) [21]. This method efficiently eliminates overshoot and avoids edge cases of both numerator and denominator being equal to 0.

3. RESULTS AND DISCUSSION

After the experimental data were preprocessed, a dataset was obtained that contained 2 input features and one target. The input features were the frequency f (Hz) and the number of loading cycles N. The target was dissipated energy W_{dis} (MJ/m^3). The dataset had 10761 samples

and comprised data for six test frequencies, namely, 0.1, 0.5, 1, 5, 7, and 10 Hz. The data were also normalised to the interval [0,1].

To build the prediction regression models, the Orange 3.38 Data Mining software was utilized.

To train the models, *k*-fold cross-validation method was employed. In the present study, *k* was chosen as 5.

In general, 4 models were built using the methods of Random Forest, AdaBoost, Gradient Boosting, and Neural Network. The training of the models was performed on a laptop with a 13th-generation Intel Core i7-1365U, with a frequency of 1800 MHz, that has ten cores and twelve logical processors, and 32 GB of RAM.

The flowchart of the model built in Orange Data Mining software is shown on Fig. 1

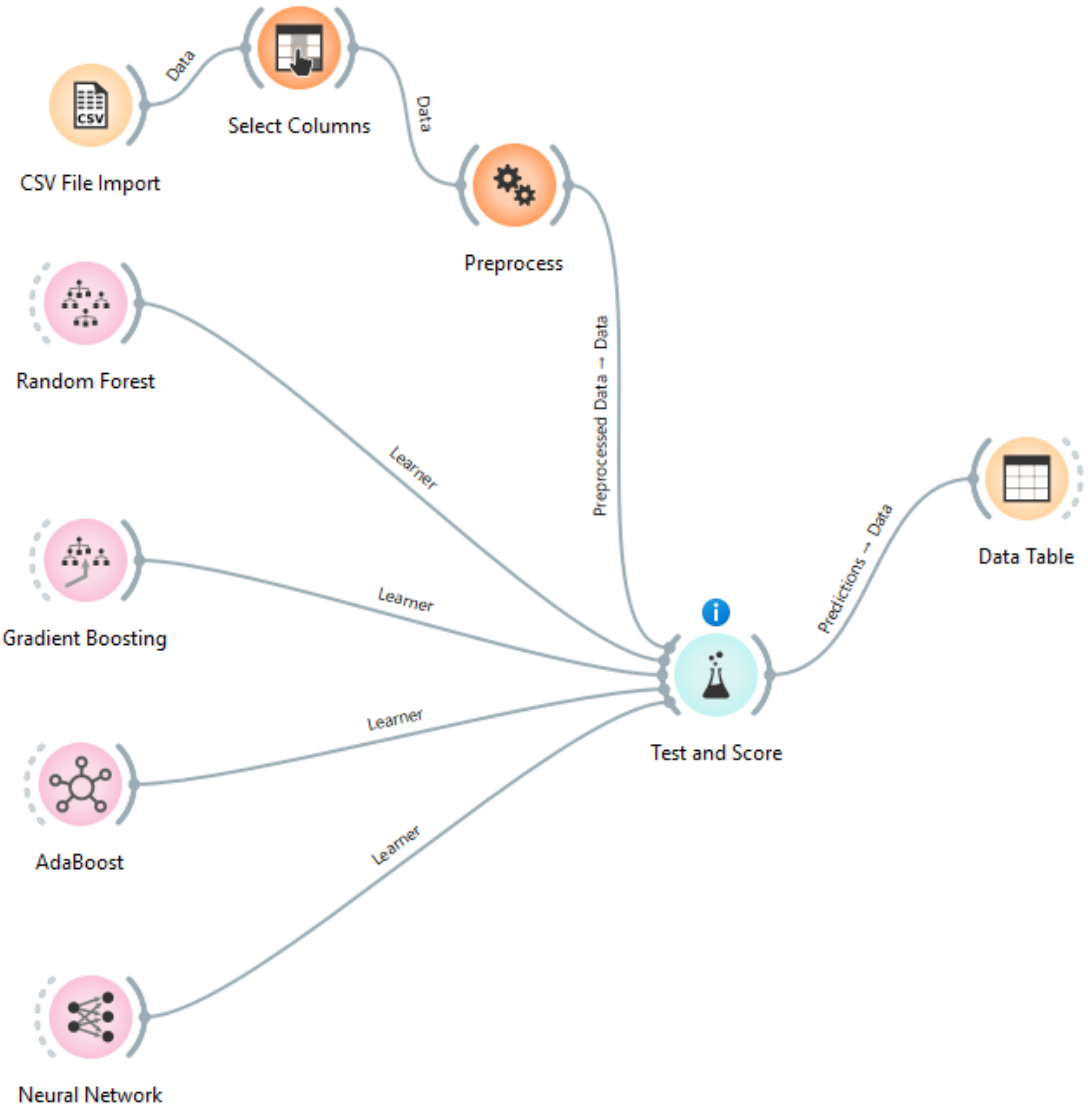

Figure1. Flowchart of the model built in Orange Data Mining Software

Table 1 shows the performance of models, and running time of the corresponding methdos.

Table 1

The performance of the models

Model	Train time [s]	Test time [s]	MSE	RMSE	MAE	MAPE
AdaBoost	2.413	0.108	10816.392	104.002	1.698	0.074
Random Forest	0.833	0.026	13377.201	115.660	2.476	0.144
Gradient Boosting	2.546	0.014	13826.829	117.588	5.595	47.103
Neural Network	17.234	0.021	13902.953	117.911	18.427	222.660

As can be seen from Table 1, the best results were shown by the ensemble methods, such as AdaBoost, Random Forest. For instance, the MAPE of AdaBoost was just 0,074, whereas the MAPE of Random Forest was 0.144. It was found that the Gradient Boosting method and Neural network are not suitable for such a dataset, since the errors are quite large and are not good enough to be employed for solving such a problem.

4. CONCLUSIONS

In the current study, the modelling of dissipated energy of NiTi shape memory alloy was performed by means of supervised machine learning methods, taking into account the test loading frequency.

The dataset contained the hysteresis curves for six loading frequencies of 0.1, 0.5, 1, 5, 7, and 10 Hz. The input data consisted of the next features: stress s (MPa), cycle number N, and loading frequency f (Hz). Based on these data, for each loading cycle, and for each loading cycle, the dissipated energy was calculated.

To remove noise, Locally Weighted Scatterplot Smoothing (LOWESS) smoother in the nonparametric package of statsmodels was utilized. After that, the trapezoid numerical integration method was employed to calculate the area enclosed by the hysteresis loop of the respective cycle, that is, the dissipated energy W_{dis}.

To augment the dataset, its points were interpolated using the modified Akima interpolation method (makima). Four models were built using the methods of Random Forest, AdaBoost, Gradient Boosting, and Neural Network.

It was found that the Gradient Boosting method and Neural Network are not suitable for such a dataset, since the errors are quite large and, therefore, these methods are not good enough to be employed for solving such a problem.

The best results were shown by the ensemble methods, such as AdaBoost, and Random Forest. For instance, the MAPE of AdaBoost was just 0.074, whereas the MAPE of Random Forest was 0.144.

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МОДЕЛЮВАННЯ ФУНКЦІОНАЛЬНИХ ВЛАСТИВОСТЕЙ SMA ЗА ДОПОМОГОЮ МЕТОДІВ МАШИННОГО НАВЧАННЯ

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Резюме. *Дослідження стосується моделювання розсіяної енергії NiTi сплаву з пам'яттю методами машинного навчання з учителем, враховуючи частоту навантаження. Сплави з пам'яттю форми – матеріали, які становлять важливий інтерес як для науки, так і для промисловості. Ці матеріали користуються широкою популярністю з огляду на їхні дві особливі властивості: унікальний ефект пам'яті форми та псевдопружність, спричинені прямим аустенітно-мартенситним перетворенням і зворотним мартенситно-аустенітним перетворенням. Традиційні детерміновані методи оцінювання властивостей матеріалу часто є дороговартісними, вимагають значних часових витрат, вимагають добре тренованого персоналу та лабораторного обладнання. На противагу цьому, за останні роки методи штучного інтелекту завоювали широку увагу через їхню здатність знаходити приховані інсайти з існуючих даних. Машинне навчання є*

частиною штучного інтелекту. Вона дозволяє вчитися на основі наявних даних і стає ліпшою з часом без явної вимоги програмування. Експериментальні дані взято з відкритих наукових джерел. Вони містили криві гістерезису для шести частот навантаження 0,1; 0,5; 1; 5; 7 та 10 Hz. Вхідні дані складалися з наступних ознак: напруження (MPa), циклу навантаження N, і частоти навантаження f (Hz). Ґрунтуючись на експериментальних даних, для кожної частоти навантаження і для кожного циклу, обчислено розсіяну енергію. Для того, аби видалити шум, скористалися Локально Зваженим Згладжування Графіка (ЛЗЗГ) з пакету nonparametric модуля statsmodels. Після цього площу під петлею гістерезису, тобто розсіяною енергію Wdis, обчислювали числово, інтегруючи методом трапецій . Для того, аби збільшити набір даних, його точки інтерполювали модифікованим методом інтерполяції Akima (makima). Побудовано чотири моделі методами випадкових лісів, Ада Буст, Градієнтним Бустінгом і нейронною мережею. Найліпші результати показали ансамблеві методи, такі, як Ада Буст і випадковий ліс. Приміром, MAPE методу Ada Буст складала тільки 0,074, тоді як MAPE випадкового лісу становила 0,144. Виявлено, що методи градієнтного бустінгу і нейронні мережі не підходять для такого набору даних, оскільки помилки є досить великими. Таким чином, ці методи недостатньо добрі для застосування до розв'язування такої задачі.

Ключові слова: *сплав з пам'яттю форми, машинне навчання, розсіяна енергія, Ада Буст, випадковий ліс, дерева прийняття рішень, наука про дані, аналіз даних, інтелектуальний аналіз даних, великі дані, задача регресії.*

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