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INVESTIGATION OF RELATIONSHIP BETWEEN MANUFACTURING PARAMETERS AND PHASE TRANSITION TEMPERATURE

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Abstract- It is known that nitinol is a promising functional material that is used in aerospace, bioengineering, medicine and other fields of modern high technologies. In this work, the dependence of the transition temperature on the processing conditions during the synthesis of NiTiHf alloy, a modification of nitinol, which has a wide application field, was investigated by using Machine Learning (ML) methods, and certain theoretical results were obtained. In addition, suggestions were made to improve the obtained results.

Keywords: Nitinol, Machine Learning, Deep Learning, Regression, Python.

1. INTRODUCTION

Over the past 30 years, materials science has made significant development in the field of data generation. As a result, huge amounts of data are collected in different data sources related to material science [1-4]. To manage and use this data effectively Big Data term was added. Big data is a collection of unstructured, semistructured and structured data accumulated by world organizations that can be extracted for information and applied in predictive modeling, machine learning projects and other advanced data science-based applications [5]. ML (Machine learning) is a field that can deal with big data and meets the requirements of scientists and engineers the in modern world. Machine learning is the science where different regression, classification or statistical algorithms are developed depending on given target and data. ML methods play an important role in solving actual problems in the field of materials science [6-11]. One of these problems is the synthesis of new types of alloys based on finding an effective relationship between various characteristics of alloys. For instance, ML is used to detect and develop alloys with narrow thermal hysteresis in parallel with the optimization of thermal hysteresis and transition temperatures.

ML methods consist of 2 main subsets: Shallow Learning and Deep Learning. Shallow learning methods belong to classic ML methods and are designed to work with relatively small amounts of data. Shallow learning methods include algorithms such as Linear Regression, Logistic Regression, Random Forest, Support Vector Machine (SVM) and Gaussian process regression. Deep learning methods refer to methods based on modified artificial neural networks and are designed to work with large-scale data. Deep learning methods include algorithms such as Multi-Layer Perceptron (MLP), Long Short-Term Memory (LSTM) Convolutional Neural Network (CNN), Recurrent Neural Network (RNN), and Deep Belief Network (DBN) [12-16].

Shape memory alloys belong to alloys that can recover their original shape and size during phase transformation. One of the most common shape memory alloys is NiTi (nitinol) and NiTi-based alloys. Nitinol consists of approximately equal amounts of Ni and Ti elements and is widely used in the development of cardiovascular stands, micro activators, and in the fields related to damping instruments. Interest to Nitinol started in 1972 when William Bulher and Frederick Wang found the shape memory effect of NiTi-based alloys during working in military laboratory [17]. Nitinol has two unique properties: thermal shape memory effect and super elasticity which makes it promising for use in various industries [18-21]. The mechanism of shape memory effect is shown in Figure 1, while mechanism of super elasticity is presented in Figure 2 [18].

Many scientific works and articles have been published in the field of synthesis of nitinol and its alloys by ML methods [22-28]. Analyzing the research conducted in this field in recent years, it can be concluded that the most important characteristics during the synthesis of nitinol are transition temperatures and thermal hysteresis. Numerous works and researches devoted to this field show that the transition temperatures during the synthesis of nitinol are affected not only by the composition of the alloy but also by its processing conditions. Gauss Process Regression was used for the synthesis of NiHiHf in [23].

The Pearson correlation method was applied to find correlation between input features and temperatures. Then thermal hysteresis and average transition temperatures were predicted with higher accuracy by using not only structural but also processing features of alloy and confirmed by physics-informed feature engineering. High results were obtained by taking into account the processing parameters of NiHiHf using artificial neural network in [24]. Unlike previous work, most of the input data features consist of processing

condition and just atomic percentage of elements in NiTiHf alloy were used in the calculation. High accuracy was gained by Neural Network as regression algorithm. Shallow learning algorithms were applied to find transition temperatures of NiTiHf [25]. Results of each method were compared among each other and discussed. Deep Learning was applied to predict the conventional yield strength, conventional tensile strength and unit elongation of binary nitinol [26]. As a result, Deep Learning showed higher accuracy compared with Random Forest which also was applied in this article.

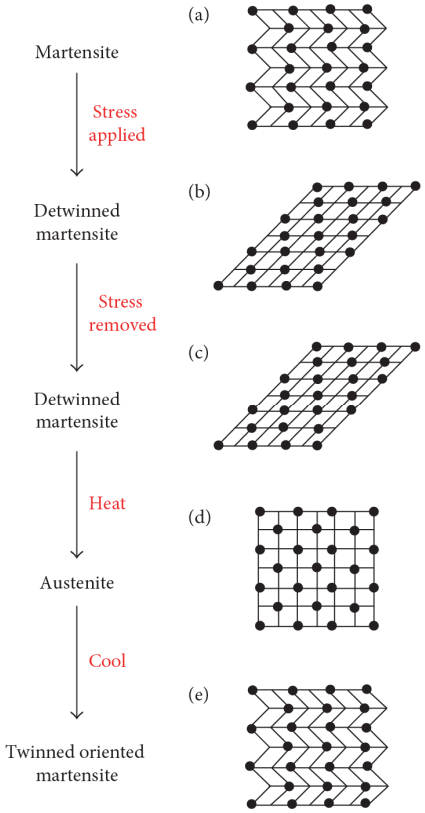

Figure 1. Mechanism of shape memory effect [28]

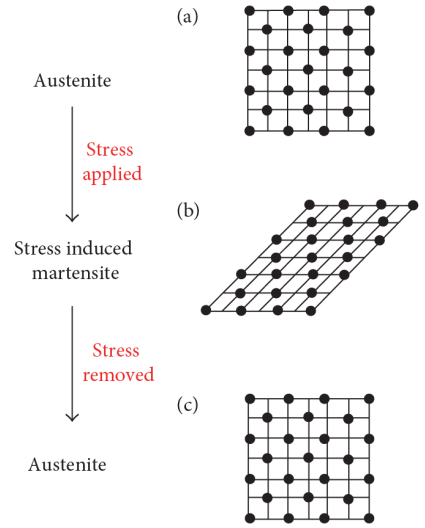

Figure 2. Mechanism of super elasticity [28]

2. EXPERIMENTAL PART

In this work, the dependence of processing conditions on the transition temperatures in an alloy based on nitinol was studied using classical ML methods. The calculations were carried out on the Jupyter Notebook online platform based on Python 3.9.1. In parallel with the classical methods of ML, the expediency of using deep learning methods (Deep Learning) is proposed. To determine the dependence of the transition temperature on the processing parameters, the data were divided into 70% (training sample for calculating the dependence) and 30% Data was taken from [28] work (Table 1).

Before starting create regression we need to better understand correlation between phase temperature and manufacturing parameters.

For that we apply Pearson correlation matrix (Figure 3). As we can see from the matrix Width and P are strongly positive correlated with A_f (0.6-0.79). E_v and Relative density have positive moderate correlation with A_f (0.4-0.59). Only Width and SS has weak positive and weak negative correlation respectively (0.2-0.39).

The data used to run the algorithms are taken from [20].

Linear regression, Support Vector Machine and Gauss Process Regression (GPR) applied as regression algorithms. The accuracy measure of algorithm is demonstrated with R^2 (Coefficient of determination) and MAE (Mean Absolute Error) which calculation formula given by [23, 29].

$$R^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \tag{1}$$

and

$$MAE = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)}{n} \tag{2}$$

where, $\hat{y}_i$ is predicted value, y_i is actual data, $\bar{y}_i$ is the mean value of output data, and i amount of data used in samples.

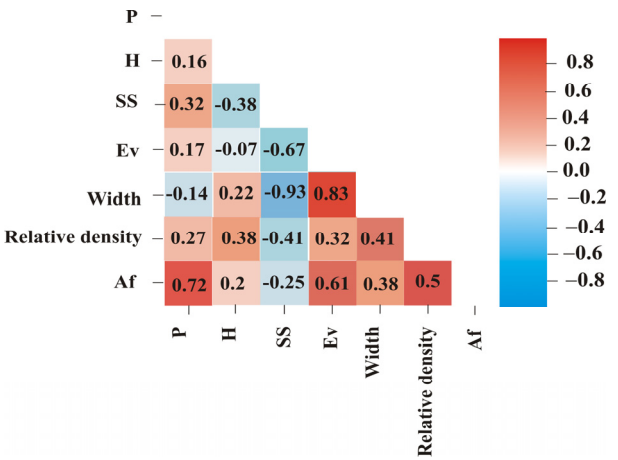

Figure 3. Pearson correlation matrix

Based on experimental and predicted data, Figure 4 and represents graphical results of regression algorithms used in train sample, while Figure 5 and illustrates graphical results of regression algorithms used in test sample. Regression results briefly showed in Table 2. Linear Regression between processing conditions and transition temperature shows R^2=83.5% accuracy and 20.06 K MAE for train data and R^2=68.4% accuracy and 41.36 K MAE for test data (Figures 3a and 4a).

Gauss Process Regression between processing conditions and transition temperature shows R^2=80.4% accuracy and 22.67 K MAE for train data and R^2=78% accuracy and 31.55 K MAE for test data (Figures 3b and 4b). Support Vector Regression between processing conditions and transition temperature shows R^2=81.8% accuracy and 19.45 K MAE for training data and R^2=74.5% accuracy and 34.82 K MAE for test data.

Linear kernel was used during regression because of higher accuracy compared to other kernel algorithms (Figures 3c and 4c). from the computed results, the higher accuracy in training sample belongs to Linear Regression. However, in test sample accuracy decreased from R^2=83.5% to R^2=68.4% and MAE from 22.67 K to 41.36 K which worst results among compared algorithms.

Table 1. Data used in regression algorithm

No.	*P* (w)	*H* (μm)	*SS* (mm/s)	*Ev* (J/mm^3)	*Width* (mm)	Relative density (%)	*Af* (°C)
1	100	140	200	119	4.72	99.96	154
2	135	120	400	93.7	4.58	99.63	256
3	210	120	400	145.8	4.6	98.39	332
4	135	80	800	70.3	4.33	96.83	143
5	175	100	600	97.2	4.61	96.82	157
6	250	120	1000	69.4	4.08	98.82	254
7	200	60	1000	111.1	4.28	97.82	276
8	100	140	400	59.52	4.42	96.98	210
9	150	60	1000	83.3	4.26	96.16	187
10	150	80	200	313	4.92	99.14	353
11	250	120	200	347.2	5.05	97.67	378
12	210	80	400	218.7	4.72	98.74	347
13	250	140	466.7	127.5	4.51	98.19	327
14	100	60	1000	55.5	4.09	91.01	119
15	250	60	1000	138.9	4.25	98.10	304
16	250	60	733.3	189.4	4.5	97.80	331
17	200	140	200	238.1	4.74	98.76	348
18	210	120	800	72.9	4.34	97.76	258
19	250	140	1000	59.5	4.09	98.08	255
20	100	60	733.3	75.7	4.38	97.68	146
21	100	80	200	208.3	4.8	97.36	144
22	100	120	200	138.9	4.78	97.87	150
23	100	60	200	277.8	4.8	98.50	280
24	210	80	800	109.4	4.41	98.24	294
25	250	140	733.3	81.7	4.36	98.24	288
26	250	60	466.7	297.7	4.66	99.20	363
27	150	140	200	178.6	4.78	98.67	332
28	250	140	200	297.7	5.95	98.52	346
29	250	80	1000	104.2	4.25	98.23	294
30	135	80	400	140.6	4.58	97.31	239

Similar to Gauss Process Regression, Support Vector Regression, shows nearly the same accuracy in both train and test samples R^2=81.9%, 19.45 K MAE and R^2=74.5%, 34.82 K MAE respectively. Obtained higher accuracy by using linear kernel emphasize that both train and test samples can be linearly separable.

Gauss Process Regression shows nearly the same accuracy in both train and test samples R^2=80.4%, 22.67 K MAE and R^2=78%, 31.55 K MAE, respectively. As a result, this algorithm is preferable than others. The obtained results show the necessity for further research in this field.

Table 2. Regression results of models

		Regression model		
Metrics (Accuracy)		svm.lin	Linear regression	GPR
	Train data	81.8%	83.6 %	80.4%
	Test data	74.5 %	68.4 %	78%
		Regression model		
Metrics (MAE)0	Data type	svm.lin	Linear regression	GPR
	Train data	19.45 K	20.06 K	22.67 K
	Test data	34.82 K	41.36 K	31.55 K

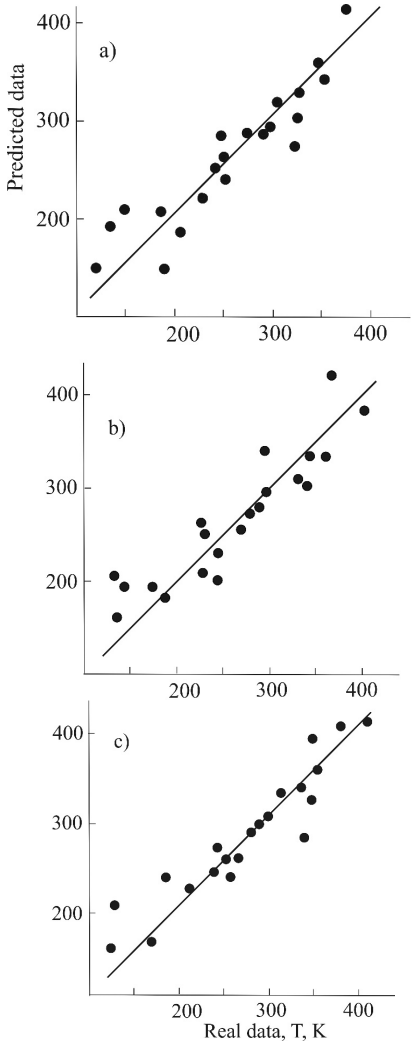

Figure 4. Regression graphs of used algorithms (train sample), (a) Linear Regression, (b) Gauss Process Regression, (c) Support Vector Regression

3. CONCLUSIONS

In this work, influence of processing conditions to transition temperature of NiTiHf alloy, was investigated by using Machine Learning (ML) methods, and gained results was compared among each other. Obtained results was demonstrated as graphs and tables. The results can be used during manufacturing of NiTi based alloys which show shape memory and super elasticity properties.

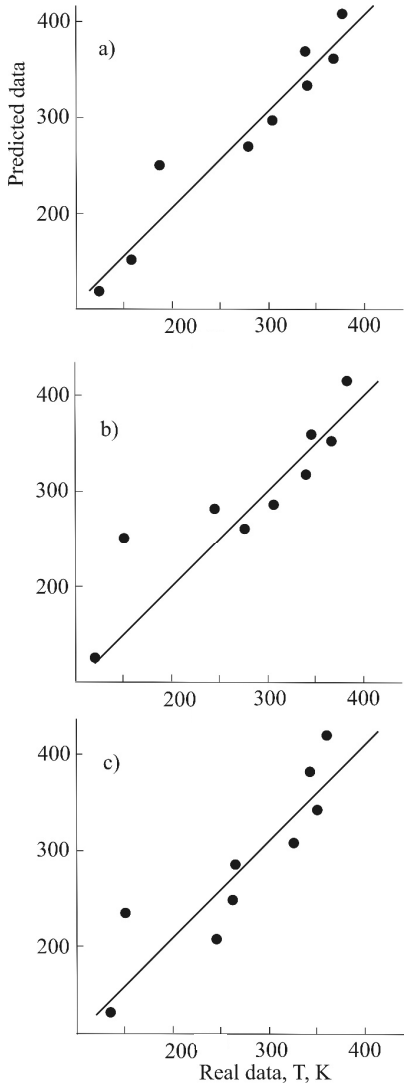

Figure 5. Regression graphs of used algorithms (test sample), (a) Linear Regression, (b) Gauss Process Regression, (c) Support Vector Regression

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