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The modelling of NiTi shape memory alloy functional properties by machine learning methods

Abstract

Shape memory alloys (SMAs) exhibit several unique properties, including superelasticity and the shape memory effect. They can return to their original shape after deformation when heated. SMAs are widely used in various fields of science and technology. Shape memory alloys are functional materials that are used under loading, which in many cases is cyclic in nature. In the present study, the functional properties of NiTi shape memory alloys were modeled using supervised learning methods. The analysis was performed using Orange data mining software, which allows the creation of visual flowcharts and the generation of results in tables and graphs. The modeling was performed on four specimens. For each specimen, several functional properties, such as residual strain range $\Delta\varepsilon_r$ and dissipated energy range ΔW_{dis}. Each data set was divided into two unequal parts - the training and test sets. The training sets comprised 66% of the total data set. The remaining 34% was used for the test set. Among the methods studied, kNN, AdaBoost, Gradient Boosting and Random Forest showed the best results in terms of prediction errors. Therefore, ML learning methods are a powerful and promising tool for solving tasks related to the prediction of functional properties of SMAs.

1. INTRODUCTION

Shape memory alloys (SMAs) exhibit several unique properties, including superelasticity and the shape memory effect. They can recover their initial shape after deformation when heated. SMAs are widely employed in various fields of science and technology. For instance, SMAs can be found even in artificial space objects (Wang et al., 2024). SMAs are being used to create actuators in biomechatronics and biorobotics (Liu et al., 2023; Popovic et al., 2019), as well as in the building of concrete structures (Dębska et al., 2021; Molod et al., 2022). Some science and technology problems can be solved through classical deterministic methods (Pogrebnjak et al., 2022; Świć et al., 2021), while others try to employ statistical or probabilistic approaches.

Machine learning (ML) is a subset of artificial intelligence (AI) that utilizes statistical methods. AI is nowadays ubiquitous (Burkov, 2019; Cabanillas-Carbonell et al., 2025; Frankiewicz et al., 2025; Hang et al., 2024; Kirda et al., 2025; Ślesicka et al., 2025; Sujana et al., 2025; Velychko et al., 2024; Yasniy et al., 2022). In general, there are three main types of ML: supervised learning, unsupervised learning, and reinforcement learning (Cabanillas-Carbonell et al., 2025; Ślesicka et al., 2025). Regression tasks are traditionally solved utilizing supervised learning. The models are trained based on data. These methods enable prediction for unknown data that the model has not seen before.

ML is a constantly evolving field consisting of many algorithms and methods that attempt to learn from available data and make predictions without being explicitly programmed. Increased computing resources, large amounts of data, and advances in statistical and algorithmic methods have made ML quite popular (Jordan & Mitchell, 2015; Lecun et al., 2015). The ML can be found almost everywhere, from the recommendation systems on the Internet (Smith & Linden, 2017; Steck et al., 2021) to medicinein medicine (Boy et al, 2025; Chen et al, 2018; Cruz & Wishart, 2007; Habti & Azmani, 2025; James & Osubor, 2025; Sirmayanti et al., 2025), Finance (Gao et al., 2024; Kelly & Xiu, 2023) or autonomous vehicles (Alfonso et al., 2024; Ravi et al., 2024).

By revealing patterns and relationships within the data, ML methods can make accurate predictions on new, unseen instances, thereby uncovering hidden patterns in the data.

Shape memory alloys (SMAs) are functional materials that are stressed, often cyclically. The degradation of SMA material properties is characterized by the energy dissipated, as there is a direct relationship between the area under the hysteresis loop and the damage to the material. Residual strain measures the ability of the material to withstand cyclic loading.

Therefore, these properties are crucial for the SMA material behavior under cyclic loading.

The aim of this study was to model the functional properties of SMAs using ML methods.

2. DATASET AND METHODS

The modeling was performed using the data mining software Orange, which allows users to visually build flowcharts of data processing algorithms and obtain results in both numerical and graphical formats.

The purpose of Orange software utilization was to build corresponding regression models based on the available experimental data. It is possible to employ various regressors from the available ones. The main role of Orange software was to train ML models.

The experimental data was in CSV files. Each file contained a number of loading cycles N, and either residual strain range $\Delta\varepsilon_r$ or dissipated energy range ΔW_{dis}. The number of cycles was treated as an input feature, and the respective functional property was chosen as a target.

Each dataset was split into two uneven parts - the training and test sets. The training sets comprised 66% of the total dataset. The remaining 34% were left for the test set.

Initially, the import file was processed via CSV file import. After that, feature selection was performed utilizing the Select Columns widget. Additionally, data preprocessing was performed to segment the range of [0, 1]. After that, a certain regressor was chosen to train the model. Afterwards, performance metrics were evaluated, and respective predictions were performed. Figure 1 shows the block diagram of the calculations.

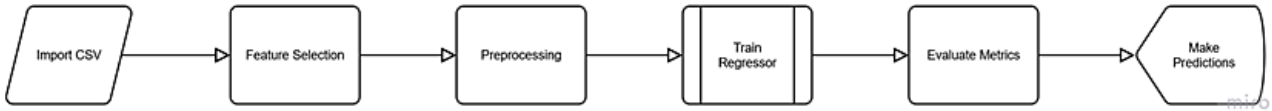

Fig. 1. The block diagram of computations in Orange data mining software

The modeling was performed on four specimens. For each specimen, several functional properties were obtained, such as the residual strain range $\Delta\varepsilon r$ and the dissipated energy range ΔW_{dis}.

Prior to modeling, the data was pre-processed. Namely, the data set was augmented by applying the Akima interpolation method (1970). This method takes into account the fast growth of the function and shows quite good results. The interpolation was performed using the Python 3 programming language. As a result of such data augmentation, one gets 1000 points for the functional property of each sample.

Figure 2 shows the flowchart of calculations in Orange data mining software.

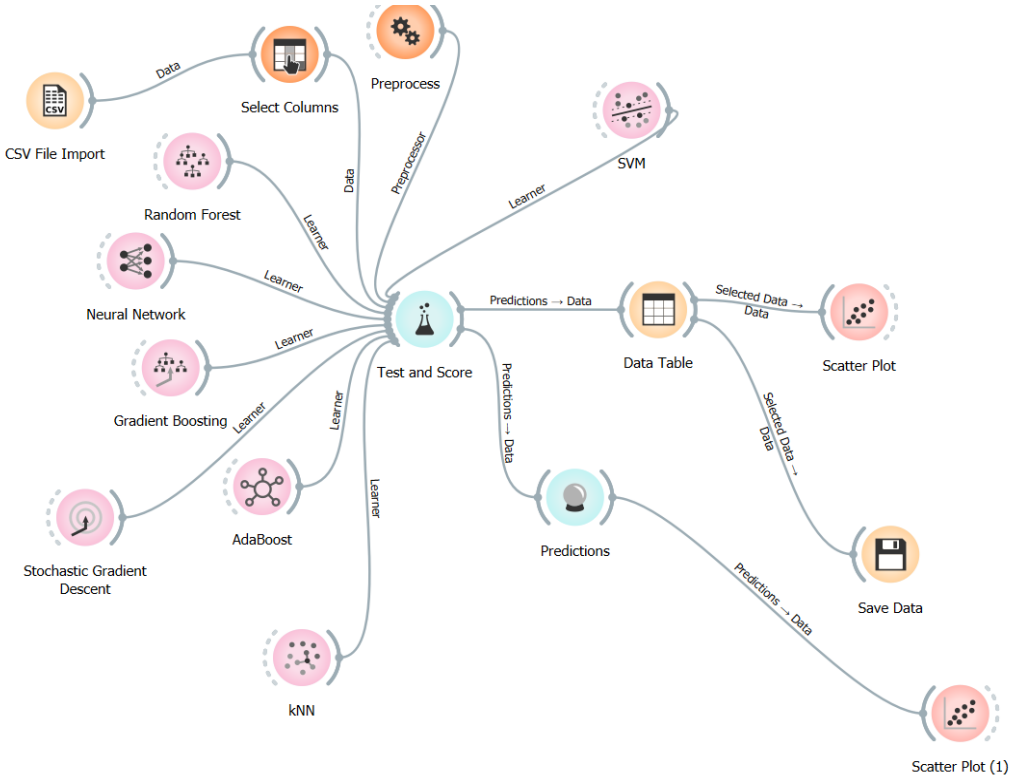

Fig. 2. The flowchart of computations in Orange data mining software

The modeling was performed using k-Nearest Neighbors (kNN), Support Vector Machines (SVMs), Stochastic Gradient Descent (SGD), Random Forest, Neural Network (NN), Gradient Boosting and AdaBoost. As a result of the modeling, the regression dependencies of the available data were obtained. In addition, a 10-fold cross-validation of the models was performed.

The kNN method is a relatively simple but robust regression algorithm. It solves the regression problem by using a similarity measure. This algorithm is a nonparametric method (Srisuradetchai & Suksrikran, 2024).

SVMs are methods based on the structural risk minimization principle of inductive learning. It works well with small sample sizes. The algorithm is based on an attempt to minimize empirical risk and the VC (Vapnik-Chervonenkis) dimension. Vapnik and his colleagues at AT&T Bell Laboratories refined the methods. SVM algorithm allows finding hidden patterns in complicated data sets (Basak et al., 2007).

The gradient descent method is one of the most widely used optimization algorithms for solving ML problems. Its stochastic version has recently received considerable attention and is mainly used to train deep neural networks (DNNs). In DNN, the gradient after a sample or a set of samples is used to avoid the consumption of expensive computational resources and saddle points. Stochastic optimization is a fundamental method used in machine learning, mainly due to the back-propagation algorithm in a neural network (NN) (Lu, 2022).

Random forest is a method developed by Leo Breiman in the 2000s that is based on an ensemble of multiple decision trees. The algorithms are remarkably effective and cope well with sparsity; their convergence speed depends only on the number of strong features and not on the number of noise variables provided.(Biau, 2012).

A classical NN consists of many simple interconnected units called neurons, each of which performs a set of activations. Input neurons are activated by sensors that sense the environment, and other neurons are activated by weighted connections from previously active neurons. Specific neurons can affect the environment by triggering actions. Learning an NN means calculating the weights that make the NN show the desired behavior (Schmidhuber, 2015).

Boosting is a method that makes it possible to build highly accurate predictions by combining several less accurate ones. Proposed by Friedman (2001; 2002) and Natekin and Knoll (2013) Gradient Boosting Machines (GBMs) are predictive models built using back-fitting and nonparametric regression. Instead of building a single model, the GBM generates an initial model and proposes new models by minimizing the loss function to obtain the most accurate model (He et al., 2019; Natekin & Knoll, 2013).

Boosting algorithms are quite different, each with its own characteristics and strengths. One of the earliest and most effective boosting methods is Adaptive Boosting (Freund & Schapire, 1997) also known as AdaBoost. AdaBoost iteratively recalculates the weights of misclassified samples, with subsequent models paying more attention to these examples.

3. RESULTS AND DISCUSSION

The data for four samples were described by the respective machine learning models. The MSE, RMSE, MAE, and R^2 were calculated for each model. The model metrics for Sample #10 are shown in Table 1.

Tab. 1. The models metrics for specimen # 10

Specimen #10	MSE	RMSE	MAE	R^2	MSE	RMSE	MAE	R^2
SVM	0.089	0.298	0.244	0.95	0.395	0.628	0.092	0.137
SGD	0.199	0.446	0.401	0.888	0.409	0.639	0.156	0.107
Random Forest	0	0.016	0.008	1	0.331	0.575	0.034	0.277
Neural Network	0.024	0.155	0.111	0.986	0.402	0.634	0.099	0.121
Gradient Boosting	0	0.018	0.013	1	0.212	0.460	0.028	0.537
AdaBoost	0	0.014	0.008	1	0.212	0.460	0.027	0.537
kNN	0	0.018	0.006	1	0.276	0.525	0.032	0.397

For the example #10, the lowest MSE was achieved by Random Forest, Gradient Boosting, AdaBoost, and kNN for the $\Delta\varepsilon_{res}$. The same is true for RMSE and MAE. These methods also gave the highest values of R2 = 1. The same picture is observed for ΔW_{dis}. The first place in terms of lowest error was taken by AdaBoost with MAE equal to 0.027. Gradient Boosting came in second with an MAE of 0.028. Third was kNN with an MAE of 0.032. Fourth place goes to SVM with an MAE of 0.092. However, the R2 values are acceptable only for the first three ML models. These results confirm that ensemble methods provide superior performance for this example.

The models metrics for specimen #13 are shown in Table 2.

Tab. 2. The models metrics for specimen # 13

Specimen #13	MSE	RMSE	MAE	R^2	MSE	RMSE	MAE	R^2
SVM	0.055	0.234	0.089	0.515	0.352	0.539	0.122	0.187
SGD	0.089	0.299	0.164	0.211	0.408	0.639	0.216	0.058
Random Forest	0.015	0.121	0.014	0.87	0.102	0.319	0.026	0.765
Neural Network	0.086	0.293	0.13	1	0.398	0.631	0.149	0.08
Gradient Boosting	0.015	0.121	0.016	0.871	0.081	0.285	0.025	0.812
AdaBoost	0.015	0.121	0.017	0.871	0.081	0.285	0.024	0.812
kNN	0.02	0.142	0.015	0.823	0.138	0.371	0.025	0.681

The same picture is observed for the sample #13 as for the sample #10. The lowest values of MSE, RMSE, and MAE were obtained by Random Forest, Gradient Boosting, AdaBoost, and kNN for the $\Delta\varepsilon_{res}$. The highest values of $R^2 = 1$ were also obtained by these methods. The slightly worse results were obtained by Neural Network, SGD and SVM. This confirms the fact that they are not suitable for this case. The same applies to Δ_{Wdis}.

The model metrics for Sample #16 are shown in Table 3.

Tab. 3. The models metrics for specimen # 16

Specimen #16	MSE	RMSE	MAE	R^2	MSE	RMSE	MAE	R^2
SVM	0.006	0.080	0.073	0.796	0.027	0.165	0.096	0.418
SGD	0.008	0.088	0.077	0.756	0.04	0.2	0.119	0.15
Random Forest	0	0.008	0.001	0.998	0.007	0.082	0.006	0.855
Neural Network	0.006	0.078	0.063	0.807	0.036	0.189	0.080	0.241
Gradient Boosting	0	0.005	0.001	0.999	0.004	0.064	0.006	0.914
AdaBoost	0	0.005	0.001	0.999	0.004	0.063	0.005	0.914
kNN	0	0.007	0.001	0.998	0.006	0.078	0.004	0.871

As for sample #16, the four methods mentioned above are the best for the two datasets studied, $\Delta\varepsilon_{res}$ and ΔW_{dis}. The lowest values of MSE, RMSE, and MAE were calculated by Gradient Boosting, AdaBoost, kNN, and Random Forest for the $\Delta\varepsilon_{res}$, and for the ΔW_{dis}. The highest R^2 values of 1 were also obtained by these methods. As for the ΔW_{dis}, the highest values of R^2 were obtained by Gradient Boosting and AdaBoost. This result confirms the high potential of this type of ML models for predicting the functional properties of SMA. Also, these two methods showed $R^2 = 0.914$, which is quite a good result.

The model metrics for sample #17 are shown in Table 4.

Tab. 4. The models metrics for specimen # 17

Specimen #17	MSE	RMSE	MAE	R^2	MSE	RMSE	MAE	R^2
SVM	0.011	0.106	0.079	0.986	0.134	0.366	0.127	0.622
SGD	0.155	0.394	0.295	0.813	0.243	0.493	0.26	0.317
Random Forest	0	0.021	0.005	0.999	0.01	0.102	0.01	0.971
Neural Network	0.003	0.059	0.027	0.996	0.017	0.131	0.046	0.951
Gradient Boosting	0	0.017	0.008	1	0.004	0.062	0.009	0.989
AdaBoost	0	0.016	0.005	1	0.004	0.062	0.008	0.989
kNN	0.001	0.024	0.004	0.999	0.011	0.103	0.01	0.97

As in the three previous cases, kNN, AdaBoost, Gradient Boosting and Random Forest gave the best results in terms of prediction errors.

From the obtained result, it can be concluded that it is advisable to use boosting methods as well as Random Forest. Also, kNN showed remarkably high results. It can also be used in engineering practice.

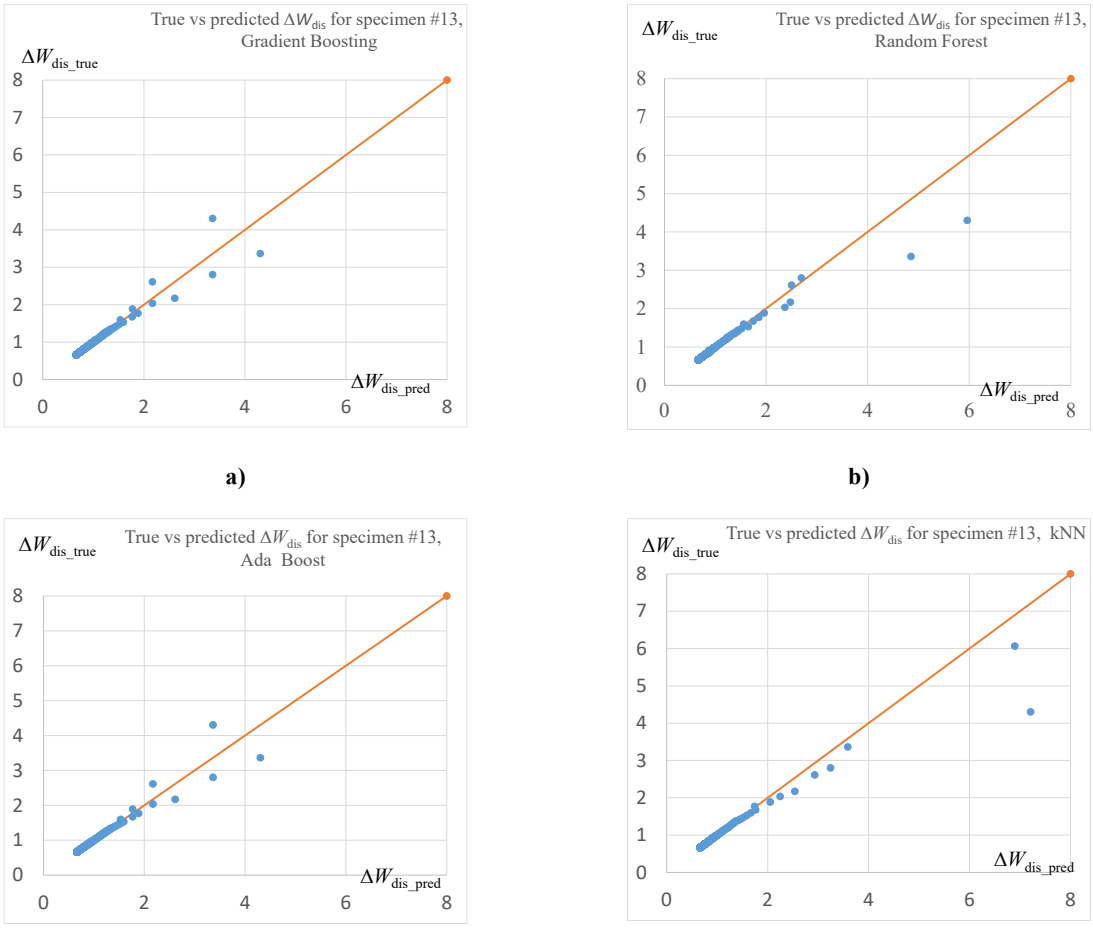

Fig. 3. The true vs. predicted dissipated energy ΔW_{dis} for specimen # 13 obtained by ML methods: a) Gradient Boosting; b) Random Forest; c) Ada Boost; 4) kNN

Fig. 3 shows the dependencies of true versus predicted dissipated energy ΔW_{dis} obtained by four ML methods with the best prediction error: a) Gradient Boosting; b) Random Forest; c) Ada Boost; 4) kNN. As can be seen from the plot, the points are close to the bisector of the first coordinate angle, confirming the high prediction accuracy.

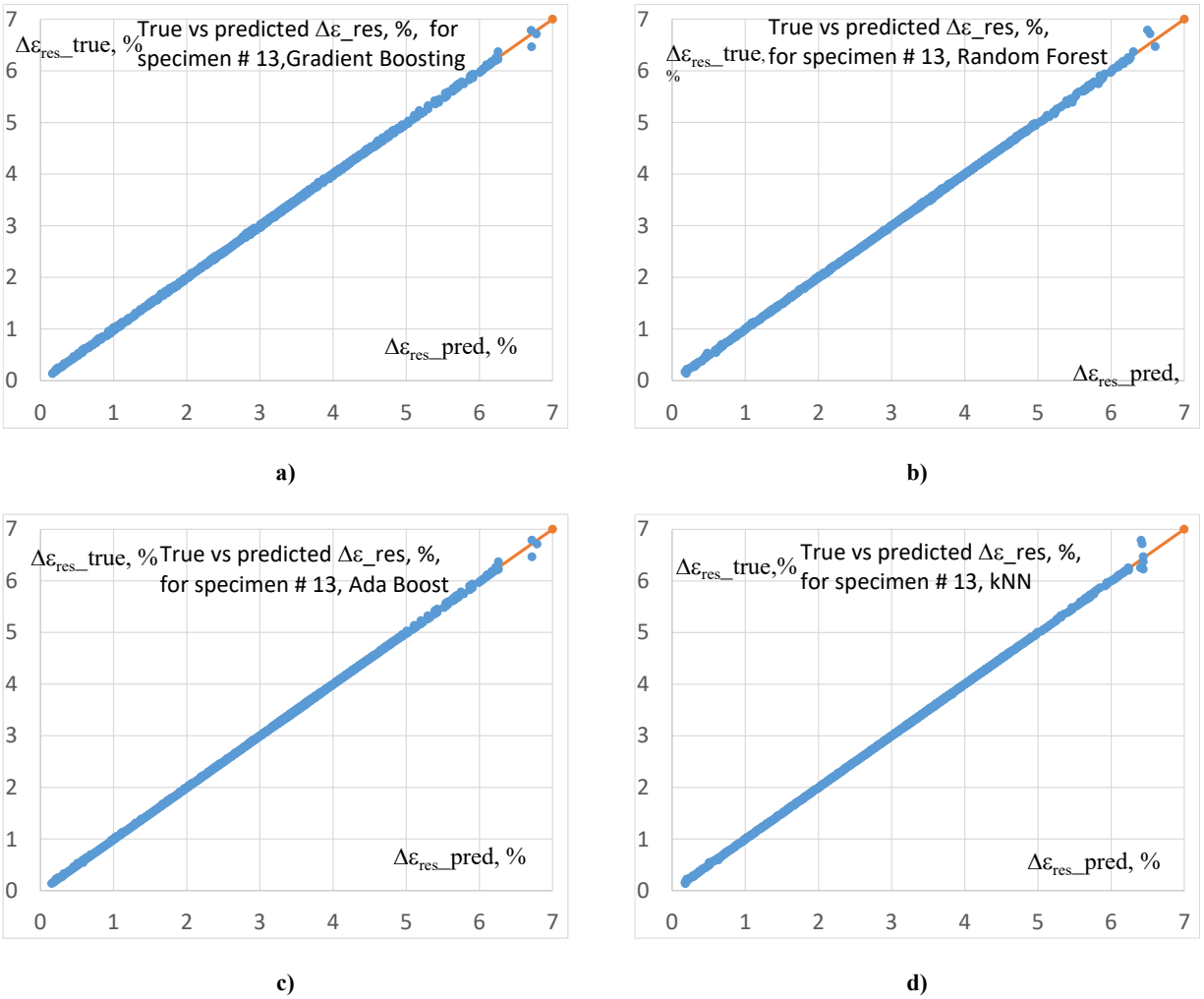

Fig. 4. The true vs. predicted residual strain $\Delta\varepsilon_{res}$ for specimen # 13 obtained by ML methods: a) Gradient Boosting; b) Random Forest; c) Ada Boost; 4) kNN

Figure 4 shows the dependencies of the true versus predicted residual strain range $\Delta\varepsilon_{ress}$ calculated by the four best ML methods in terms of prediction error: a) Gradient Boosting; b) Random Forest; c) Ada Boost; 4) kNN. As in the previous case, the points on the plot are close to the bisector of the first coordinate angle, indicating high prediction accuracy.

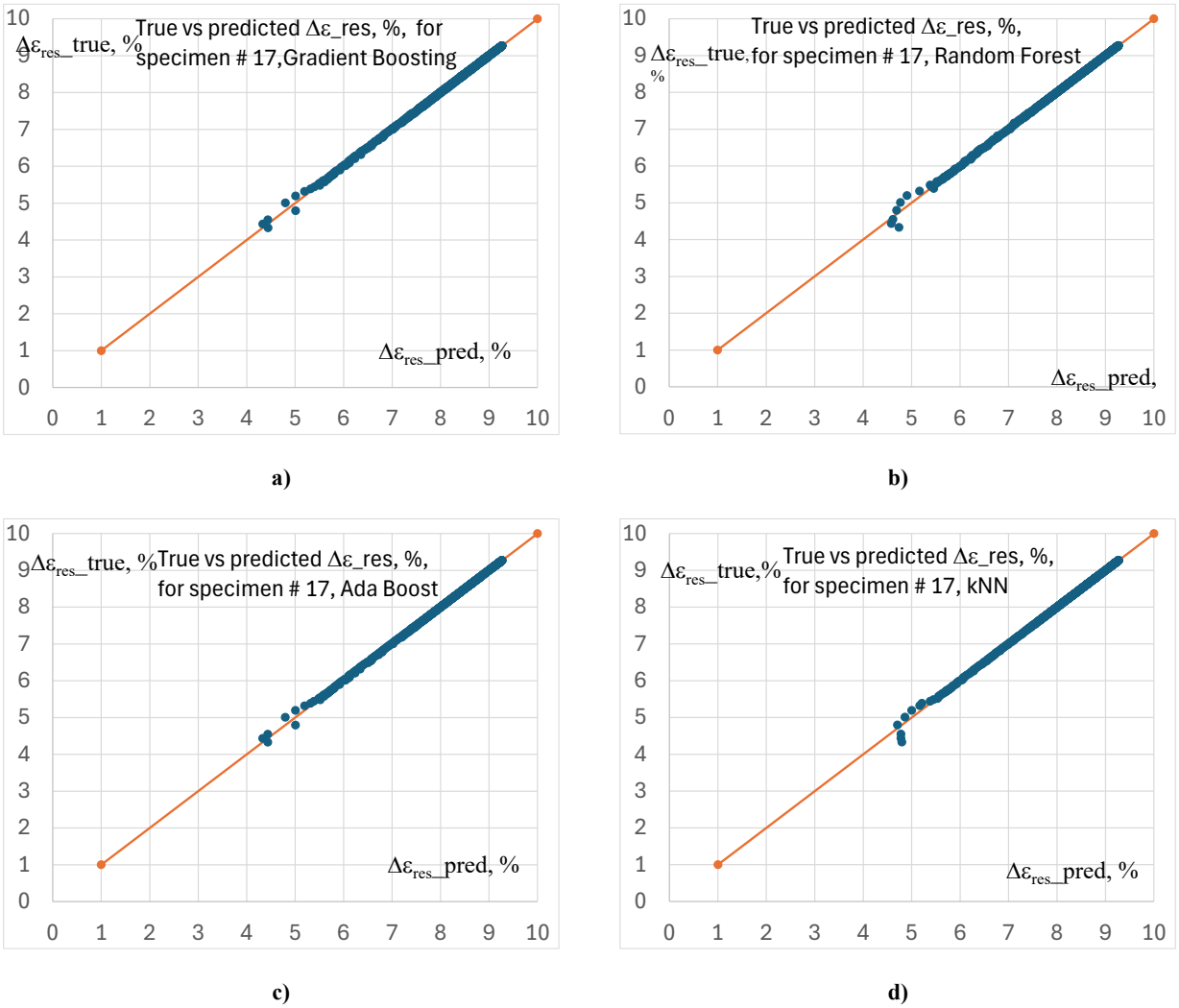

Fig. 5. The true vs. predicted residual strain $\Delta\varepsilon_{res}$ for specimen # 17 obtained by ML methods: a) Gradient Boosting; b) Random Forest; c) Ada Boost; 4) kNN

Figure 5 shows the dependence of the true versus predicted residual strain range $\Delta\varepsilon_{ress}$ obtained by the four best ML methods in terms of prediction error: a) Gradient Boosting; b) Random Forest; c) Ada Boost; 4) kNN. As in the case of sample 17, the points on the plot are very close to the bisector of the first coordinate angle, confirming the low prediction error and therefore high prediction accuracy.

4. CONCLUSIONS

During the study, the functional properties of NiTi shape memory alloys were modeled using supervised machine learning methods. The modeling was performed on the Orange data mining platform. As a result, the regression dependencies of the residual strain and dissipated energy ranges for the four specimens studied were obtained using the k-Nearest Neighbors (kNN) method, as well as Support Vector Machines, Stochastic Gradient Descent method, Random Forest methods, Neural Networks, Gradient Boosting and AdaBoost. Among the methods studied, kNN, AdaBoost, Gradient Boosting, and Random Forest showed the best results in terms of prediction errors. This demonstrates the high potential of ensemble models in predicting the areas of dissipated energy and residual strain. Therefore, ML learning methods are a powerful and promising tool for solving tasks related to the prediction of functional properties of SMAs. In future research, it is planned to use model stacking to further improve the predictive power with respect to the functional properties of SMA.

Conflicts of interest

The authors declare no conflict of interest.

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