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RESEARCH PAPER

PREDICTION OF HARDNESS, FLEXURAL STRENGTH, AND FRACTURE TOUGHNESS OF ZrO_2 BASED CERAMICS USING ENSEMBLE LEARNING ALGORITHMS

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ABSTRACT

Flexural strength, hardness, and fracture toughness are the basic mechanical properties of ceramic materials. Manufacturers widely use this set of properties to ensure the durability of ceramic products. However, many factors, such as chemical and phase compositions, sintering temperature, average grain size, density, and others, affect these properties, making it challenging to estimate corresponding reliability parameters correctly. Experimental examination of the impact of these factors on the mechanical properties of ceramics is a rather time-consuming and resource-consuming procedure. This work aims to predict the mechanical properties of zirconia ceramics using machine learning tools. The authors have created an experimental database for predicting the hardness, flexural strength, and fracture toughness of ZrO_2-based ceramics based on chemical composition, phase composition, microstructural features, and sintering temperature on the mechanical properties of zirconia ceramics. To solve this problem, we compared the effectiveness of using five single machine learning algorithms and five ensemble methods of different classes. We found a high accuracy of the predicted values of each of the three mechanical properties using ensemble methods from the boosting class (CatBoost, AdaBoost, and XGBoost). The authors developed a stacked ensemble of machine learning methods to improve the accuracy of determining the hardness property prediction task. The effectiveness of linear and nonlinear meta-regressors in the scheme of the developed ensemble is investigated. We obtained an increase in accuracy of more than 10% (R^2) using our approach.

Keywords: ceramics; prediction task; hardness; flexural strength; fracture toughness; machine learning, ensemble methods, small data approach

INTRODUCTION

Recently, many manufacturers of ceramic products (Metoxit AG (Switzerland), Yamakin Co. Ltd. (Japan), Dentsply Sirona (USA), Amann Girrbach AG (Austria), Morgan Advanced Materials (UK), and CERAM TEC (Germany) [1]) have provided customers with a wide range of precision products manufactured according to their needs, while ensuring sufficient durability of the products. Yttria stabilized zirconia (ZrO_2-Y_2O_3), due to its high flexural strength and fracture toughness, is widely used for various applications [2–4]. The mechanical properties of ceramics based on ZrO_2 are close to those of stainless steel [2,5,6]. Products made of such ceramics can operate under high temperatures, high pressure, corrosion, and friction conditions. Yttria stabilized zirconia ceramics are widely used for the manufacture of bearings [7], friction plates, valve plates, ball valves, pipeline linings, nozzles, directional drilling tool components, control valves, pump plungers, metering pump parts, moulds, protective tubes of thermocouples, solid oxide fuel cells [8–12] and thermal protective coatings [9,10,13]. Zirconia is widely used to manufacture internal combustion engine components (bearings, rollers, dies, pushers, valves, and fuel injectors) [14,15].

The use of ceramics based on ZrO_2 in biomedicine began at the end of the 20th century [16]. The use of zirconia in dentistry has recently increased significantly due to the demand for metal-free restorations [17–22]. Ceramics should have high flexural strength to operate stably in the environment of the oral cavity for a long time [23]. Flexural strength is a critical mechanical characteristic determining the possible clinical use of ceramics in tooth restoration [24–26]. Compared to other dental ceramics, ceramics doped with Y_2O_3 provide the highest flexural strength [16,18,27]. Y-TZP ceramics also have high fracture toughness due to implementing the transformation strengthening mechanism [2,10,20,28–32]. A successful combination of high flexural strength and fracture toughness, aesthetics, and biocompatibility made it possible to manufacture zirconia-fixed partial dentures and single-tooth reconstructions, which successfully replaced metal ones [23,28,30,33–37]. Endodontic pins, crowns and bridges [38], restorations and abutments for implants [24,33,39], aesthetic orthodontic brackets [40], and post systems [33] are

made of such ceramics. Due to higher fracture toughness and lower modulus of elasticity, zirconia is increasingly used to replace ceramics based on Al_2O_3 to manufacture implant-supported restorations [20,24,26]. The highly transparent Y-TZP ceramic with high purity and almost zero porosity (Zirconia system Zenostar from Wieland Dental) is characterized by high optical and mechanical properties and increased resistance to hydrothermal aging [41]. Wear resistance, characterized by hardness, is also one of the critical mechanical characteristics of ceramics, which determines the durability of finished products [15].

The results of orthopaedic studies have proven that zirconia ceramics can be used to manufacture femoral head prostheses instead of titanium or alumina prostheses [2,28,34,42]. The mechanical properties of the monolithic zirconia restorative material are significantly superior to other all-ceramic restorative materials. However, some authors [33,41,43–45] report the disadvantages of zirconia anterior restorations, which are associated with fractures and chips due to the high sensitivity to brittle fracture of zirconia implants. Therefore, zirconia ceramics stabilized by yttrium are used mainly for monolithic restorations of corner teeth monolithic posterior restorations, which made it possible to increase fracture resistance significantly [46].

The main task of scientists is to propose ways to improve the mechanical properties of zirconia ceramics, namely flexural strength, hardness, and fracture toughness, which will significantly increase the durability and operating life of finished products.

Based on the review of scientific literature and our research, an experimental database was created, which shows the influence of chemical composition, phase composition, microstructure features, and sintering temperature on the mechanical properties of zirconia ceramics. Experimentally determining these parameters' influence on flexural strength, hardness, and fracture toughness is a rather long and resource-consuming process. Therefore, machine learning methods were used to predict the mechanical properties of zirconia ceramics.

The main contribution of this paper can be summarized as follows:

- We collected three datasets of mechanical properties for ZrO_2-based ceramics, which take into account the chemical composition, phase composition, microstructural features, and sintering temperature;
- We investigated the effectiveness of five ensemble machine learning methods and five single machine learning algorithms in solving the problems of predicting three mechanical properties of zirconia ceramics. Experimentally, we have established a satisfactory prediction accuracy of all three studied mechanical properties by ensemble machine learning methods;
- We have developed a new stacked ensemble of four machine learning methods to improve the accuracy of predicting the hardness of ZrO_2-based ceramics. We have investigated the effectiveness of using different meta-regressors in the developed stacking ensemble. The prediction accuracy was increased by more than 10% using nonlinear meta-regressors compared to the most accurate existing method (XGBoost).

The structure of this paper is the following. Section 2 describe the process of data collection. Research methodology as well as proposed stacking approach is described in section 3. Modeling process as well as obtained results is presented in section 4. Section 5 describe the results of comparison and discussion. A summary of the obtained results is presented in the Conclusions section.

DATA COLLECTION

Chemical composition is a base characteristic of ceramics. In general, it determines the type of chemical bonds formed between particles of initial powders during ceramics production. It is well known that oxide ceramics are defined as a group of ceramics containing not more than 15% silica with little or no glass phase [47].

It is known that the structure of an advanced ceramic is under control on macrostructural and microstructural levels electronic and atomic levels and grain boundaries. This critical feature is considered when fabricating porous and dense ceramic materials with a refined microstructure. It should be noted that other features also affect the performance of ceramic materials, e.g., crystal structure, grain size, defect types and their chemical composition, and the nature of the impurities and their distribution [48]. Paper [49] studied YSZ ceramics stabilized with 3, 4, 5, 6, 7, and 8 mol% Y_2O_3, which were sintered at 1550 °C for 2 h. It was shown that fracture micro mechanism operating in fine-grained microstructures with a comparatively high percentage of the monoclinic (m) ZrO_2 phase is the most favourable for practical applications. This micro mechanism, implemented in 7YSZ ceramics, shows the highest level of flexural strength and fracture toughness, as the crack propagates along the boundaries of the agglomerates of fine grains and occasionally cleavage through larger grains occurs. The last ones may be enriched with yttrium and have a cubic (c) or partially stabilized tetragonal (t) crystal structure. In this paper, Y_2O_3, MgO, CeO_2, Al_2O_3, TiO_2, and other complementary oxides were considered dopants for ZrO_2 based ceramics. Such a variety of dopant oxides allows for achieving different mechanical and functional properties of materials. Thus, the role of each of them in the formation of ZrO_2 based ceramics flexural strength, hardness, and fracture toughness should be evaluated quantitatively and in terms of prevalence over other oxides.

Phase composition is one of the essential characteristics of ceramics. It is especially crucial for ZrO_2 based ceramics in which a tetragonal to monoclinic (t-m) phase transformation may occur under external loading and other concomitant factors. On the one hand, the phase composition of a ceramic material directly relates to its chemical composition. On the other hand, it depends to a great extent on a sintering mode (i.e., sintering temperature, dwell time, heating/cooling rate, etc.). Three phases, namely cubic and/or tetragonal and/or monoclinic, can be formed in ZrO_2 based ceramics doped with various oxides. Paper [50] studying ZrO_2 based ceramics revealed that the t-ZrO_2 phase became more stable when the average grain size decreased, particularly when values of this parameter became smaller than 0.3 μm. Such a value was set as a critical one. At smaller values of the average grain size, the t-ZrO_2 phase was found to stabilize at ambient temperature [51].

It was reported for ZrO_2 based ceramics with the addition of 5.29 wt% Y_2O_3 and 0.005 wt% Al_2O_3 [52] that the t-m transformation and, as a result, transformation strengthening of the material was retarded by non-uniform distribution of Y_2O_3, intensive grain growth at high sintering temperatures, as well as high percentage of c-ZrO_2 formed under these conditions. Papers [53–55] noted that the studied YSZ ceramics with 2-3 mol% Y_2O_3 contained a significant percentage of the tetragonal phase and showed the highest trend towards transformation strengthening. It was also reported in [37] on the microstructure of widely used in dentistry ZrO_2 based ceramics formed by 0.3–0.4 μm grains of the tetragonal phase. Other authors [56] showed that the grain size in tetragonal zirconia stabilized with yttrium after sintering for 2 h at 1550 °C was 0.3–0.7 μm.

Paper [57] investigated the effect of the ZrO_2 percentage on the fracture toughness and flexural strength of Al_2O_3–ZrO_2 ceramics. They detected α-Al_2O_3 and the monoclinic and tetragonal ZrO_2 phases in the studied ceramics. With a gradual increase in the total ZrO_2 percentage, the t-ZrO_2 percentage decreased. It was shown that retardation in the growth of Al_2O_3 crystals was

reached due to adding 10–20% ZrO_2, thus improving the ceramics' mechanical properties.

Therefore, each of the three zirconia phases (cubic, tetragonal, and monoclinic) was analysed regarding its domination in corresponding ceramic material.

The sintering temperature is a parameter that provides energy for the consolidation of initial powders due to the interdiffusion of elements on the particle interfaces [58–61]. Corresponding bonds are formed between particles of initial powder, followed by their recrystallization. It positively affects the flexural strength and fracture toughness of ZrO_2 based ceramics. Paper [62] showed that ZrO_2 ceramics containing 5% Y_2O_3, <2% HfO_2, and <1% (Al_2O_3 + SiO_2) had the smallest grain size of 0.07 μm. In contrast, ZrO_2 ceramics containing 4–6% Y_2O_3, <1% Al_2O_3, max 0.02% SiO_2, max 0.01% Fe_2O_3, and max 0.04% Na_2O had the largest grain size of 0.35 μm. The authors found a correlation between the grain size in the studied ceramics, and their sintering temperature, namely 0.35 μm was after sintering at 1600 °C and 0.07 μm after that at 1350 °C.

Paper [63] reported that 3YSZ ceramics sintered at 1550 °C showed about 17% higher flexural strength than 6YSZ ceramics sintered at 1450 °C. They suggested that lower concentrations of Y_2O_3 might be positively considered in terms of the mechanical properties of such ceramics. The higher temperature of sintering these ceramics also improves the ceramics' flexural strength, hardness, and fracture toughness.

Thus, the sintering temperature is an important parameter allowing the formation of a set of microstructural components with certain morphology in ZrO_2 based ceramics ensuring their optimal flexural strength, hardness, and fracture toughness.

The average grain size of ZrO_2 based ceramics is the parameter that relates to its phase composition and sintering mode [64]. However, trends in a change of grain size for these ceramics with an increase/decrease in a separate phase fraction and an increase/decrease in a sintering temperature are ambiguous.

Paper [65] reported results on the transformation toughening of ZrO_2 ceramics stabilized with 3–4 mol% Y_2O_3. They found that the spontaneous t-m transformation does not occur in a microstructure with nano-sized grains, and the stress relaxation does not follow. Another study [66] showed that the ZrO_2 ceramic becomes unstable and prone to spontaneous t-m transformation with increased grain size. Such transformation may occur in this material at the crack tips and in the material bulk resulting in stress relaxation. The authors showed that the morphology and size of microstructural components, especially pores, and grains, depend to a great extent on the sintering mode. They performed mechanical tests of the ceramics and revealed a maximum flexural strength of 904 MPa for material sintered at 1580 °C. However, SEM images of the microstructure did not exhibit a significant difference in the grain size of the ceramics sintered at 1580 °C for 10 min and at 1510 °C for 120 min.

Therefore, this parameter is relevant for characterizing the mechanical behaviour of ZrO_2 based ceramics.

The density of ceramics is an important characteristic that allows indirect evaluate its density-related parameters such as porosity, relative density, etc. It is essential to consider the size, shape, and specific proportion of pores since they mainly affect the density of ceramics. Paper [67] studied the relative density of ZrO_2 with three mol% Y_2O_3. They found that with an increase in the temperature and holding time, values of this parameter increased and reached 95% and 99% after sintering for 50 h at 1300 °C and 1500 °C, respectively. The same trend was observed for the average grain size. The values of this parameter for the ceramics after holding for 50 h in a temperature range of 1300–1500 °C were 0.2–0.9 μm. The fraction of the cubic phase grew from 11 to 15 wt% at 1300 °C and from 15 to 19 wt% at 1500 °C during holding for 10 h. Further exposition at these temperatures did not cause a discernible change in the phase fractions of the ceramics.

The above-mentioned density-based parameters are used for estimating the sintering kinetics and evaluating the probability of microcrack nucleation and reduction of the lifetime of ceramic products. Therefore, density is relevant to be used for assessing the hardness, flexural strength, and fracture toughness of ZrO_2 based ceramics.

Accordingly, the database features were the oxide fractions (ZrO_2, Y_2O_3, MgO, CeO_2, Al_2O_3, TiO_2, HfO_2, SiO_2, and others), the average grain size, density, and sintering temperature were represented by numerical values. In this case, the numerical values were related to the following units: mol% for the oxide fractions, μm for the average grain size, $g \cdot cm^{-3}$ for density, and °C for the sintering temperature. Data for phase composition (cubic and/or tetragonal and/or monoclinic zirconia phase) were transformed into a binary system as follows: 1 corresponds to the dominant phase, and 0 indicates other phases. A schematic representation of the initial database for modelling is given in **Fig. 1**.

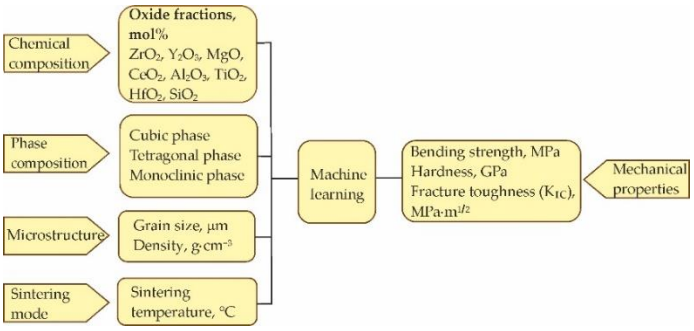


Fig. 1 Schematic representation of the initial database for modelling

MATERIAL AND METHODS

This section describes the machine learning methodology used in the paper, and the developed stacked ensemble of machine learning methods.

Machine learning methods

The modern development of Computational Materials Science is based on artificial intelligence tools. Information accumulated over the years about a particular object of observation allows

them to be used to predict/categorize its future states. Regression analysis using machine learning methods provides the possibility of preliminary modeling to minimize computational human or time and material resources for manufacturing a product. Determining the functional properties of a material or its quality characteristics by modeling with artificial intelligence methods before it is created also minimizes the use of precious raw materials, particularly in the case of the possible defective material.

A considerable arsenal of machine learning methods for analysing various data exists today. In most cases, single machine learning algorithms do not provide satisfactory forecast accuracy, which imposes several limitations on their practical application. It is due to many independent attributes that should be considered during the analysis, complex nonlinear relationships within the available dataset, and the available minimum training sample size since data in this area is expensive and time-consuming to collect.

Developing an ensemble approach to building machine learning methods has become widespread to improve prediction accuracy in recent years. The four classes of ensemble methods, boosting, bagging, stacking, and cascading have been used in various application areas to solve multiple data mining tasks.

This paper is devoted to studying the effectiveness of ensemble methods for solving the problem of predicting the mechanical properties (hardness, flexural strength, and fracture toughness) of ZrO_2-based ceramics. This choice is explained by a number of their advantages, in particular [68]:

- Reducing errors of the ensemble machine learning method compared to every single model that forms it;
- Significant improvement of forecast accuracy by combining forecasts of several models instead of one;
- Possibility to increase the generalization properties of machine learning methods by using heterogeneous algorithms in an ensemble approach, each of which is based on different data characteristics;
- The ability to reduce or even avoid the problems of overlearning or underearning that are typical for single-based machine learning methods:
- Scalability by adding auxiliary models to the ensemble.

Among the disadvantages of the ensemble approach are usually the complexity of its implementation and the need for large computing resources. Given that the experimental data in materials science are primarily small, such problems will not arise when using ensemble approaches in this work.

The authors focused their work on the most popular among the existing methods, namely [69]:

- AdaBoost;
- CatBoost
- XGBoost;
- Random Forest;
- Gradient Boosting.

Let's look at the principles and advantages of each of them.

Gradient Boosting is an ensemble machine learning method from the boosting algorithms class. It is based on the principle of iterative improvement of the method by adding "weak" models to the ensemble. Gradient Boosting works by trying to find new models that will be able to analyse better the parts of the data set where the current model performs poorly. Among the advantages of Gradient Boosting are high prediction or classification accuracy, reduced sensitivity to noise components, and the ability to work efficiently with large data sets.

Adaptive Boosting (AdaBoost) is one of the most famous ensembles of machine learning methods from the boosting class. It is widely used to solve both classification and regression tasks. The AdaBoost method is based on training a sequential series of weak models over a given dataset. After each iteration, the model assigns a weight to each data point, depending on how well it was predicted/classified. Each subsequent model focuses on the data points that were miscategorized. Among the advantages of AdaBoost is its high accuracy. In addition, unlike Gradient Boosting, AdaBoost is characterized by adaptability to changes in the data set and the ability to avoid retraining.

Categorical Boosting (CatBoost) is a Gradient boosting method explicitly developed for working with categorical variables in data. CatBoost is based on finding the optimal weights and dividing the data into "leaves" that improve the prediction at each training step. The method uses the joint work of decision trees and ensembles them to get the best result. Among the advantages of the CatBoost method are the automatic processing of categorical variables, low probability of overfitting, and support for parallel data processing with the ability to flexibly adjust model parameters.

XGBoost (eXtreme Gradient Boosting) is a type of Gradient boosting method explicitly developed to increase the speed and efficiency of similar algorithms. The XGBoost method combines several independent models built one after the other and supported by gradient boosting. At each step of the Gradient boosting, the model tries to improve the previous result and increase the forecasting accuracy. The advantages of the XGBoost method are high speed, particularly on large datasets, high prediction accuracy, and atomic selection of model hyperparameters.

Random Forest is a machine learning method that belongs to the class of bagging methods. It uses an ensemble of different trees that divide the input data into many smaller parts, thus solving the problem of overfitting that often arises when working with a single decision tree. The Random Forest method combines the results of many trees to obtain a more accurate result. Each tree randomly selects a subset of the input data and the functions used to divide the data into smaller groups. After each tree is built, they are combined for the overall result. Among the advantages of the Random Forest method are high prediction accuracy on large and small data samples, no need for feature selection procedures, and resistance to random errors.

This paper will use these methods to solve the following research objectives.

Proposed stacking approach

Suppose the training data set is short enough, and several existing machine learning methods provide adequate prediction models. In that case, the overall prediction accuracy can be improved by fusing machine learning methods [70]. This class of machine learning methods has gained wide popularity in recent years due to the ease of implementation, the intuitive nature of this approach, and the good results they provide.

Stacking machine learning methods is an approach used to combine different types of predictive models with improving prediction accuracy [71]. In stacking, low-level predictive models (base models) are used to create new features for a higher-level model, making it possible to consider more information during prediction.

The principle of stacking is as follows. A set of prediction models is selected, trained on the training sample, and the results of their work form a new dataset, where the features are the outputs of each of the low-level prediction models [68]. This dataset is used to train the meta-algorithm, which is mostly based on linear machine learning methods. The result obtained by the meta-algorithm is the value to be determined.

The scientific literature distinguishes between homogeneous and heterogeneous stacked ensembles. A heterogeneous stacked machine learning method is an approach that combines predictive

models of different types to obtain the best result [68]. Heterogeneous stacking models should use models based on different algorithms, which can increase the prediction accuracy.
Due to the limited size of the training dataset, in this paper, we propose to build a stacking model where the selection of a set of low-level models is based on the criterion of the maximum value of the coefficient of determination [68]. For example, if some single machine learning algorithms demonstrate a determination coefficient R^2>0.7, they will be selected to form a set of basic lower level regressors.
The choice of a meta-algorithm for training a higher-level stacking model will also be based on the same criterion. Here, both linear and nonlinear models can be used. Typically, linear meta-algorithms are used in the scientific literature. They are very fast and can increase accuracy by 2-3%. In this paper, along with linear, we will use and test the effectiveness of nonlinear models. This approach is justified by the fact that a nonlinear model as a meta-algorithm can significantly improve prediction accuracy. Since we are talking about processing short datasets, its training time will not significantly affect the performance of the stacking ensemble in general.

RESULTS

This section presents the numerical characteristics of the datasets used in this work. The results of studies on the effectiveness of using ensemble machine learning methods for predicting flexural strength, hardness, and fracture toughness are presented. A stacked ensemble was built based on the selection of the most accurate machine learning methods, and the use of linear and nonlinear methods as meta-regressor in the proposed ensemble was investigated.
The modeling was performed using Orange software [72]. This decision was made due to the simplicity and convenience of performing both intellectual analysis and visualization of the results obtained in this environment.
The accuracy of the studied methods was evaluated using commonly used performance indicators: MSE, RMSE, MAE, and R^2 [68]. The results' reliability was achieved using the 5-fold cross-validation option of the Test and Score widget of the Orange software environment.

Dataset description

As described in the previous section, the authors collected datasets for predicting the hardness, flexural strength, and fracture toughness of ZrO_2-based ceramics. Since, for many observations, the values of hardness, flexural strength, or fracture toughness were missing, and the attributes Grain size and Density contained a significant number of missing values, such observations were removed from the dataset. Therefore, the size of the collected data set for each property of ZrO_2-based ceramics was different. The difference in the number of observations could reach two or more times, so we considered predicting three properties of ZrO_2-based ceramics as three separate tasks. Thus, we obtained three data sets for predicting hardness, strength, and fracture toughness, respectively.
In particular, the dataset for predicting the hardness of ZrO_2-based ceramics contains 68 observations and 15 attributes. It is available in the ResearchGate repository [73].
The dataset used to predict the flexural strength of ZrO_2-based ceramics contains 33 observations and 15 attributes. It is available in the ResearchGate repository [74].
The dataset for predicting the fracture toughness of ZrO_2-based ceramics contains 80 observations and 15 attributes. It is available in the ResearchGate repository [75].
These three datasets were used to study the effectiveness of applying machine learning tools in solving the stated task.

Investigations of the existing ML method for prediction properties

Single machine learning methods do not always provide sufficient accuracy to be used in practice. An ensemble of machine learning methods can be used to avoid this problem. The small size of the collected data for analysis also justifies this choice.

General flowchart of the investigations existing ML method

Fig. 2 shows a general flowchart of the procedure for modeling and investigating the effectiveness of various machine learning methods for solving each of the three tasks of this study.

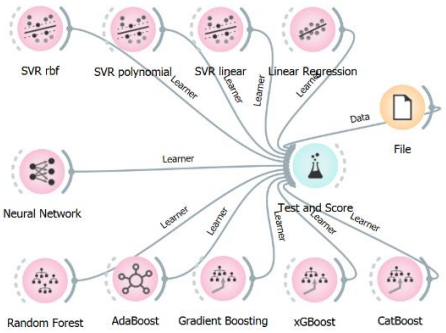


Fig. 2 General flowchart of the modeling process

In addition to the ensemble methods, we also investigated the possibility of using some well-known single machine learning methods, shown in **Fig. 2.** We used linear regression, support vector machines with different kernels and a neural network as a universal approximator.
It should be noted that all these machine learning methods were used to solve each of the three tasks. The optimal parameters of their work are shown in **Table 1**.

Fracture toughness property prediction results of ZrO_2 based ceramics

The modelling results using all the studied machine learning methods for predicting the fracture toughness property of ZrO_2-based ceramics are presented in Table 1. Since we are talking about the analysis of small data sets, the duration of the training procedures for all the studied methods was not considered.

Table 1 Performance indicators for predicting fracture toughness property of ZrO_2 based ceramics by all investigated methods

ML-based method	MSE	RMSE	MAE	R^2
CatBoost	0.963	0.982	0.726	0.70
AdaBoost	1.082	1.040	0.714	0.66
Random Forest	1.277	1.130	0.818	0.60
Gradient Boosting	1.330	1.153	0.886	0.58
XGBoost	1.451	1.205	0.910	0.55
Linear regression	1.917	1.384	1.074	0.40
SVR rbf	1.953	1.398	0.983	0.39
SVR linear	2.367	1.539	1.092	0.26
Neural Network	3.114	1.765	1.126	0.03
SVR polynomial	6353.594	79.709	15.777	-1987.37

As can be seen from **Table 1**, several ensemble methods have been used to predict the fracture toughness of ZrO_2-based ceramics with sufficient accuracy. In addition, the neural network as a universal approximator also provided a high prediction ac-

curacy. The highest prediction accuracy, in this case, was obtained using the CatBoost algorithm. It reaches 70% according to the coefficient of determination (R^2).

Flexural strength prediction results of ZrO_2 based ceramics

The performance indicators for predicting the flexural strength of ZrO_2-based ceramics using all the studied machine learning methods are given in **Table 2**.

Table 2 Performance indicators for prediction flexural strength of ZrO_2 based ceramics by all investigated methods

ML-based method	MSE	RMSE	MAE	R^2
AdaBoost	23982.681	154.863	102.368	0.77
Gradient Boosting	26008.552	161.272	97.282	0.75
Random Forest	31361.96	177.093	136.282	0.70
CatBoost	31589.968	177.736	129.061	0.69
Neural Network	35878.783	189.417	1467.486	0.65
XGBoost	38835.797	197.068	132.565	0.62
Linear regression	63414.302	251.822	186.174	0.39
SVR linear	83207.59	288.457	238.939	0.19
SVR polynomial	103184.746	321.224	274.056	0.01
SVR rbf	105450.314	324.731	279.01	-0.02

As seen from **Table 2**, in this case, ensemble prediction methods from both boosting and bagging classes also demonstrated high prediction accuracy. However, the highest accuracy of the flexural strength prediction for ZrO_2-based ceramics was obtained using the AdaBoost algorithm. It reaches 77% (according to the coefficient of determination).

Hardness property prediction results of ZrO_2 based ceramics

The accuracy of predicting the hardness property of ZrO_2-based ceramics using all the studied machine learning methods is shown in **Table 3**.

Table 3 Performance indicators for prediction hardness property of ZrO_2 based ceramics by all investigated methods

ML-based method	MSE	RMSE	MAE	R^2
XGBoost	2.562	1,60	0,960	0,79
Neural Network	2.726	1,65	1,218	0,78
CatBoost	2.816	1.68	0.974	0.77
Random Forest	3.322	1.82	1.086	0.73
Gradient Boosting	4.710	2.17	1.242	0.61
Linear regression	6.037	2.46	1.710	0.51
AdaBoost	6.414	2.53	1.273	0.47
SVR polynomial	6.784	2.61	1.709	0.44
SVR linear	7.366	2.71	1.808	0.40
SVR rbf	10.059	3.17	1.892	0.18

As can be seen from the obtained results, in this case, as in the two previous ones, the ensemble methods constructed an adequate prediction model with acceptable results. In particular, the highest prediction accuracy of the hardness property of ZrO_2-based ceramics (at almost 80%) was obtained using the XGBoost algorithm.

The results of the application of the proposed ensemble

Generally, improved prediction accuracy in small data processing can be achieved using stacked homogeneous or heterogeneous ANNs.

General flowchart of the proposed approach

Fig. 3 shows a flowchart of the modeling procedure according to the stacking ensemble proposed in this paper. First, it should be noted that it was developed to increase the prediction accuracy of the hardness property of ZrO_2-based ceramics. This is due to the sufficient size of the dataset to implement this approach.

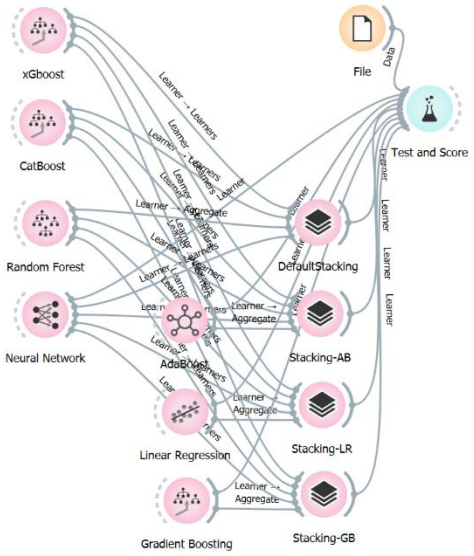


Fig. 3 General flowchart of the proposed stacking approach

The stacking of machine learning methods was performed, considering their accuracy. In particular, the proposed ensemble included those methods from all the studied ones that demonstrated a determination coefficient value of more than 0.7. As can be seen from the previous table, these methods include XGBoost, Neural Network, CatBoost, and Random Forest.
In addition to choosing weak regressors for the first step of the stacking ensemble procedure, in this paper, we investigated the impact of using different meta-regressors for the second step of the stacking training procedure. For this purpose, we used traditional linear methods (Linear regression, Ridge regression) and nonlinear machine learning methods (Adaboost and Gradient Boosting).

Results of applying different meta-regressors in the proposed ensemble

As a result of the construction of the new ensemble method, we investigated 4 variants of the stacking combination of four machine learning methods. They differed only in the meta-regressor used during the second step of the training procedure (Linear regression, Ridge regression (Default stacking), Adaboost and Gradient Boosting). The performance indicators for applying the developed algorithms to solve the problem of predicting the hardness property of ZrO_2-based ceramics are presented in **Table 4.**

Table 4 Performance indicators for prediction hardness property of ZrO_2 based ceramics by different stacking algorithms

ML-based method	MSE	RMSE	MAE	R^2
Stacking with Adaboost	1.311	1.145	0.688	0.893
Stacking with Gradient Boosting	1.378	1.174	0.778	0.887
Default Stacking	2.034	1.426	0.917	0.833
Stacking with Linear regression	2.109	1.452	0.88	0.827

As seen from **Table 4**, the nonlinear machine learning methods used as a meta-regressor significantly increase the accuracy of the developed stacking ensemble compared to the use of linear meta-regressors.

COMPARISONS AND DISCUSSION

In this section, we present the results of comparing all the studied methods in solving the problems of predicting the mechanical properties of ZrO_2-based ceramics, namely, hardness, flexural strength, and fracture toughness.

Comparison of the fracture toughness property predicted results by different ML-based methods

The results of comparing the accuracy of different machine learning methods based on the coefficient of determination and standard deviation in solving the fracture toughness property prediction task are shown in **Fig. 4**.

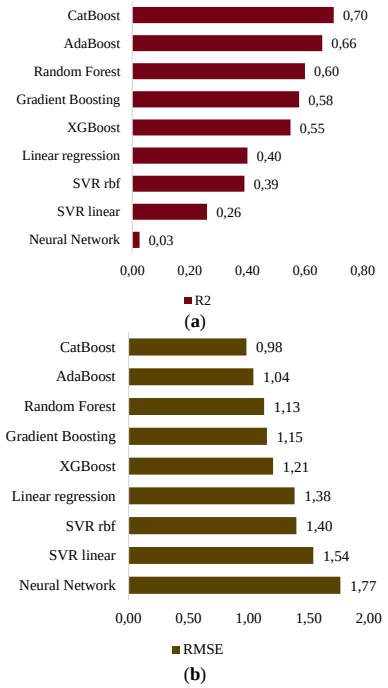


Fig. 4 Comparison of the fracture toughness property prediction task results using all investigated methods based on: (**a**) R^2; (**b**) RMSE

As can be seen from **Fig. 4**, the existing single methods demonstrate the inadequacy of the prediction models built on their basis. In this case, the coefficient of determination is below 0.5. The studied ensemble methods from different classes demonstrate different accuracy results. In particular, the XGBoost method demonstrates the adequacy of the model but the unsatisfactory prediction accuracy.
The highest prediction accuracy for the fracture toughness property of ZrO_2-based ceramics was obtained using the CatBoost algorithm. It reaches 70%. Further improvement of the prediction accuracy of this mechanical property is possible by increasing the training dataset.

Comparison of the flexural strength predicted results by different ML-based methods

The results of comparing the accuracy of different machine learning methods based on the coefficient of determination and standard deviation when solving the flexural strength prediction task are shown in **Fig. 5**.

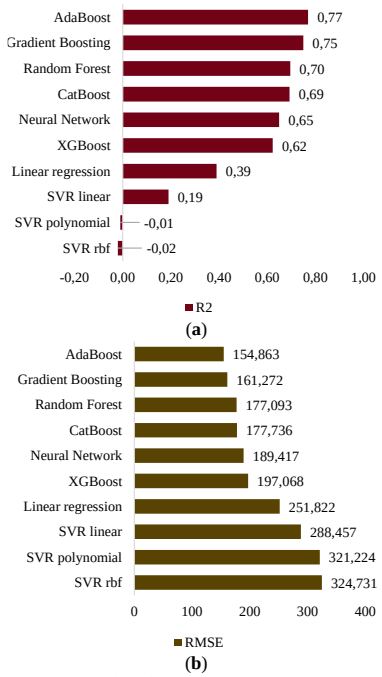


Fig. 5 Comparison of the flexural strength prediction task results using all investigated methods based on: (**a**) R^2; (**b**) RMSE

As can be seen from **Fig. 5**, the existing single methods (except Neural Network) demonstrate the inadequacy of the prediction models built on their basis. In this case, the coefficient of determination is significantly lower than 0.5.
The studied ensemble methods from different classes demonstrate different accuracy results. In particular, the XGBoost method demonstrates the adequacy of the built model but the unsatisfactory prediction accuracy at 62%.
The highest prediction accuracy for the flexural strength of the ZrO_2-based ceramics was obtained using the AdaBoost algorithm. It reaches 77%, which is quite sufficient for solving this task. Further increase in the prediction accuracy of this mechanical property is possible by increasing the training dataset.

Comparison of the hardness property predicted results by different ML-based methods

The results of comparing the accuracy of different machine learning methods based on the coefficient of determination and standard deviation when solving the hardness property prediction task are shown in **Fig. 6**.
As shown in **Fig. 6**, the studied ensemble methods from different classes demonstrate satisfactory forecasting results. In particular, four of the researched methods provide more than 70 % accuracy, and the most accurate method, XGBoost, provides a prediction accuracy of 79 %.

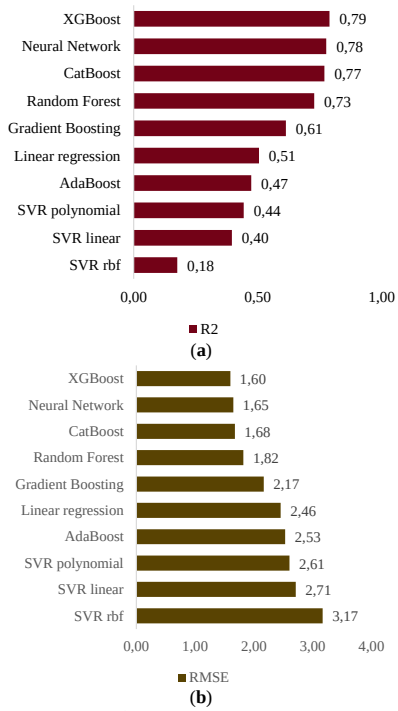
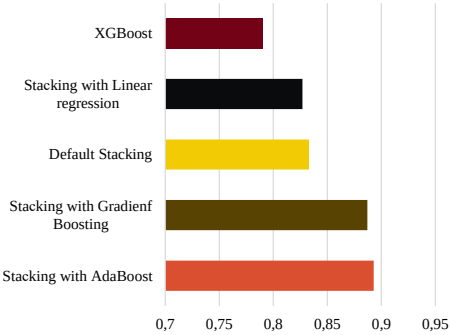


Fig. 6 Comparison of the hardness property prediction task results using all investigated methods based on: (**a**) R^2; (**b**) RMSE

In general, the following conclusions can be drawn from the results of comparing the prediction accuracy of three mechanical properties by existing machine learning methods:
In most cases, single machine learning algorithms do not provide the ability to build an adequate model for predicting each of the three properties of ZrO_2-based ceramics;
The high accuracy of the prediction of all three properties of ZrO_2-based ceramics was obtained by ensemble methods;
Random Forest, as a representative of the bagging class of ensemble machine learning methods, also provides sufficient prediction accuracy. Still, different ensemble algorithms from the boosting class obtained the highest prediction accuracy for all three properties.
Fig. 7 shows the results of comparing the algorithms developed by the authors for building a stacking model with the most accurate existing machine learning method for solving the hardness property prediction task.
As can be seen from **Fig. 7**, the use of linear meta-regressors in the developed stacking ensemble increases accuracy compared to the existing XGBoost. In particular, the use of Linear regression provides an increase in accuracy by 3.7%. The use of Ridge regression as a more accurate algorithm than the previous one as a meta-regressor provides a 4.3 percent increase in prediction accuracy compared to XGBoost. However, if we use nonlinear machine learning methods as meta-regressors in the stacking ensemble proposed by the authors, the accuracy of solving the hardness property prediction task increases significantly. In particular, Gradient Boosting increased accuracy by 9.7% compared to the existing XGBoost and by 5.4% compared to stacking based on Ridge regression as a meta-regressor.

The developed stacking ensemble based on the AdaBoost algorithm demonstrated the highest prediction accuracy as a meta-regressor. It allowed us to increase the prediction accuracy by more than 10% compared to the existing machine learning method. In general, the prediction accuracy of the hardness property at the level of 90% allows the use of the developed stacked ensemble in practice.



	Stacking with AdaBoost	Stacking with Gradienf Boosting	Default Stacking	Stacking with Linear regression	XGBoost
R2	0,893	0,887	0,833	0,827	0,79

Fig. 7 Comparison of the hardness property prediction task results using all investigated stacked algorithms based on: (**a**) R^2; (**b**) RMSE

Given the much smaller amount of available data, it does not seem appropriate to use the developed stacking ensemble or to build a similar one according to the criterion described in this work for predicting the other two mechanical properties of ZrO_2-based ceramics for training. In particular, the dataset for predicting the flexural strength of ZrO_2-based ceramics is 1.5 times smaller than the one under study. The training set for predicting fracture toughness is almost three times smaller. For the intellectual analysis of such critically small amounts of data, other strategies should be used, in particular [76–79]:

- Data augmentation with the selected tools followed by intelligent analysis using machine learning methods based on a significantly larger amount of training data;
- Ensemble methods using one or two General Regression Neural Networks or SGTM neural-like structures with nonlinear input extension based on various algorithms of the "input doubling methods";
- Homogeneous stacked ensembles of Artificial Neural Networks (without training or with non-iterative machine learning) based on the random deviation method. All these will be the focus of our further research.

CONCLUSION

This work has studied microstructure-related mechanical properties of ZrO_2 based ceramics. Chemical and phase compositions, sintering temperature, average grain size, and density influence the microstructure and, as a result, base mechanical properties such as hardness, flexural strength, and fracture toughness of ceramic materials. The impact of each factor on these properties may be different and depends on which of the property is being analysed.
The tasks of determining mechanical properties using traditional methods are quite a resource-, time-, and man-consuming. In this paper, the authors propose using artificial intelligence tools to

solve the problem of predicting the mechanical properties of zirconia ceramics using machine learning tools. For this purpose, the authors collected three datasets to predict the hardness, flexural strength, and fracture toughness of ZrO_2-based ceramics based on chemical composition, phase composition, microstructural features, and sintering temperature on the mechanical properties of zirconia ceramics. The data was cleaned and prepared for applying artificial intelligence methods.

The modeling was performed using the Orange software. For this purpose, the authors selected five well-known single machine learning methods and five ensemble methods from different classes.

The authors found high accuracy in predicting mechanical properties using the existing ensemble methods. However, the highest accuracy for hardness, flexural strength, and fracture toughness prediction tasks was obtained using different boosting ensembles. In particular, CatBoost provided 70% accuracy in predicting the fracture toughness property, AdaBoost - 77% in predicting the flexural strength, and XGBoost - 79% in predicting the hardness of ZrO_2-based ceramics.

We have performed a study to determine the effectiveness of using five single machine learning algorithms and five ensemble methods from different classes to solve the problem. The high predicting accuracy was determined for every three mechanical properties using ensemble methods from the boosting class (CatBoost, AdaBoost, and XGBoost). In addition, the authors developed a stacked ensemble of machine learning methods to improve the accuracy of solving the hardness property prediction task. The effectiveness of linear and nonlinear meta-regressors in the developed ensemble is investigated. It was experimentally established that the accuracy of solving the hardness property prediction task could be increased by more than 10% (R^2) using the developed stacking ensemble with a nonlinear meta-regressor at its core (89%).

Experimental studies have confirmed the effectiveness of the proposed stacking ensemble in solving the task. However, the authors found that the use of linear meta-regressors to implement the second step of training the proposed ensemble increases the accuracy of solving the problem by 2-4%, while nonlinear meta-regressors, AdaBoost, provide an increase in accuracy of more than 10% according to the coefficient of determination. The 90% accuracy level allows for applying the developed approach in practice.

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