

Modeling of ferroelectric properties of KNN-based ceramics

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Abstract

Replacement of highly noxious lead zirconate titanate based materials in MEMS applications for environmentally safe materials remains an important task. Complex multicomponent doping of KNN ceramics provides for a significant improvement of their ferroelectric properties. The efficiency of different machine learning (ML) methods in the prediction of piezoelectric coefficient of KNN-based ceramics has been analyzed. ML integration allows one to accelerate the development of new materials and identify latent interdependences between their composition, structure, and properties. To understand the mechanisms of relationship between the composition and properties, we used the Sure Independence Screening and Sparsifying Operator (SISSO) method in combination with regression ML methods, such as Support Vector Regression, Ridge, Lasso, Elastic Net, Xtreme Gradient Boosting, Random Forest, Gradient Boosting Regression, and Extreme Tree Regression. The Gradient Boosting Regression (GBR) method proved to be the most efficient in combination with SISSO. The test sampling accuracy reached 81 %, and GBR validation for experimental data delivered a mean absolute error of 26 pC/N.

Keywords

KNN ceramics, ferroelectric properties, machine learning, Sure Independence Screening and Sparsifying Operator, Gradient Boosting Regression

1. Introduction

Potassium sodium niobate pertains to lead-free environmentally safe materials and is a potential candidate for the replacement of noxious materials in MEMS applications. However, achieving a performance comparable with that of lead zirconate titanate remains a complex task. Empirical methods of improving the performance (chemical modification, varying synthesis conditions, and post-syn-

thesis treatment) are quite time- and resource-consuming. This raises the necessity of resource-saving approaches.

The integration of machine learning (ML) into materials science allows one not only to accelerate the development of new materials but also to identify latent interdependences between their composition, structure, and properties. Machine learning algorithms have already proven their efficiency in the development of ferroelectric materials on the basis of BaTiO₃ and K_{1/2}Na_{1/2}NbO₃ [1–4].

Authors of works [1–3] showed that the Goldschmidt tolerance factor, atomic volume, electronegativity, ionic radius, atomic weight, and atomic number of elements are the key factors in the prediction of their ferroelectric properties. Algorithms for the prediction of such properties of barium titanate ceramics as piezoelectric coefficient [1, 4] and remanent polarization [2] have already been implemented. The use of the Support Vector Regression (SVR) method was successfully demonstrated in the prediction of piezoelectric modulus of BaTiO₃ based ceramics [4]. ML was used for maximizing the density of energy accumulation by lead-free barium titanate based dielectrics in weak electric fields [5]. Dielectric constants of polymers and their co-polymers were determined [6, 7]. The Curie temperature of Perovskite ceramics was predicted [8]. A regression model was used for the prediction of remanent polarization in ferro- and antiferroelectric materials PMN-PT, BT, and (K,Na)NbO₃ (KNN) ceramics [2]. Extreme Tree Regression (ETR) demonstrated good accuracy in comparison with other d_{33} prediction algorithms due to its capability of operating with small data arrays and minimizing repeated learning [9, 10]. For example, ETR [9] is also used for the prediction of the piezoelectric coefficient d_{33} of KNN ceramics.

Existing works have mostly dealt with the application of specific ML algorithms, rather than their combinations with other methods. This complicates the interpretability of modules and understanding the improvement mechanisms of ferroelectric properties. Further development in this field should target the improvement of data processing methods and the development of combined models where ML algorithms would be used jointly with physical principles.

The Sure Independence Screening and Sparsifying Operator (SISSO) method is a powerful tool for the retrieval of physically meaning descriptors [11]. The SISSO

method is used for the generation of complex features based on an initial data array, and for the identification of more relevant descriptors. This allows reducing the number of features and selecting the most appropriate ones for the target variable. Reducing the number of features is of special importance for small data sets where the excessive number of features reduces the quality of the model when the number of samples is small. This method combines high accuracy with interpretability and is used, e.g., for the prediction of polarization [12].

The aim of this work is to compare the efficiency of different ML methods in the prediction of piezoelectric coefficients of KNN-based ceramics. The SISSO method is used in combination with regression methods such as Support Vector Regression, Ridge, Lasso, ElasticNet, Xtreme Gradient Boosting (XGBoost), Random Forest (RF), Gradient Boosting Regression, and Extreme Tree Regression.

2. Machine learning-based design of KNN-based ferroelectric ceramics

2.1. Data sets and feature pool

The data set used in this work is based on the literary data containing measurement data for the macroscopic piezoelectric coefficient d_{33} of KNN ceramics and includes 152 doped compositions [13–45].

The target variable was d_{33} , the list of features being compiled taking into account the parameters of elements that affect the crystal structure (dimensional parameters, such as ionic radius, atomic weight and volume)

Table 1. Initial features

Characteristics	A -site	B -site	Reference
Effective ionic radii	r_A	r_B	[48]
t	$t = \frac{r_A + r_0}{\sqrt{2(r_B + r_0)}}$		[49]
μ	$\mu = r_B/r_0$		
Volume of atom	V_A	V_B	[50]
Atomic weight	AW_A	AW_B	
Nuclear charge effective (Slater)	NC_A	NC_B	
Distance from core electron (Schubert)	DCE_A	DCE_B	
Distance from valence electron (Schubert)	DVE_A	DVE_B	
Electron affinity	EA_A	EA_B	
Moment nuclear magnetic	MN_A	MN_B	
Valence electron number	NV_A	NV_B	[51]
Electronegativity (Pauling)	EN_A	EN_B	

and crystallochemical properties (coordination number, electronegativity as a parameter determining the type of chemical bond, etc.). The fundamental features of elements used in this work were also used earlier in other studies of ferroelectrics [2, 4, 9, 10, 12, 46, 47]. The data set contains 22 initial features, the list of which is presented in Table 1.

2.2. SISSO method for d_{33}

At the first stage, the features were calculated on the basis of the initial parameters of elements separately for the A and B sites using Eqs. (1) and (2), respectively:

$$X_A = \sum_{i=1}^n f_i X_{Ai}, \quad (1)$$

$$X_B = \sum_{i=1}^n f_i X_{Bi}, \quad (2)$$

where n is the number of atoms in the A/B sites of the Perovskite structure and f_i is the atomic fraction of each of the ions.

At the second stage the SISSO method was used for finding the effective highly significant for d_{33} descriptors. We obtained 11 descriptors, the list of which is presented in Table 2.

Table 2. SISSO descriptors

Features	Formula
f_1	$MN_B \times AW_B + V_A \times AW_A$
f_2	$DVE_B \times DCV_B + (VN_A - NC_A)$
f_3	$MN_B \times DVE_B - V_B$
f_4	$MN_B \times V_A$
f_5	$DCE_A \times NC_A - DCE_A \times V_A$
f_6	$VN_A + NC_A - DCE_A \times V_A$
f_7	$EN_B \times EA_A - EA_B \times EN_A$
f_8	$\mu + EN_A - t \times DVE_A$
f_9	$\mu + EN_A - DCE_A \times r_A$
f_{10}	$\mu + EN_A - t + DCE_A$
f_{11}	$t - NC_A + DCE_A + V_A$

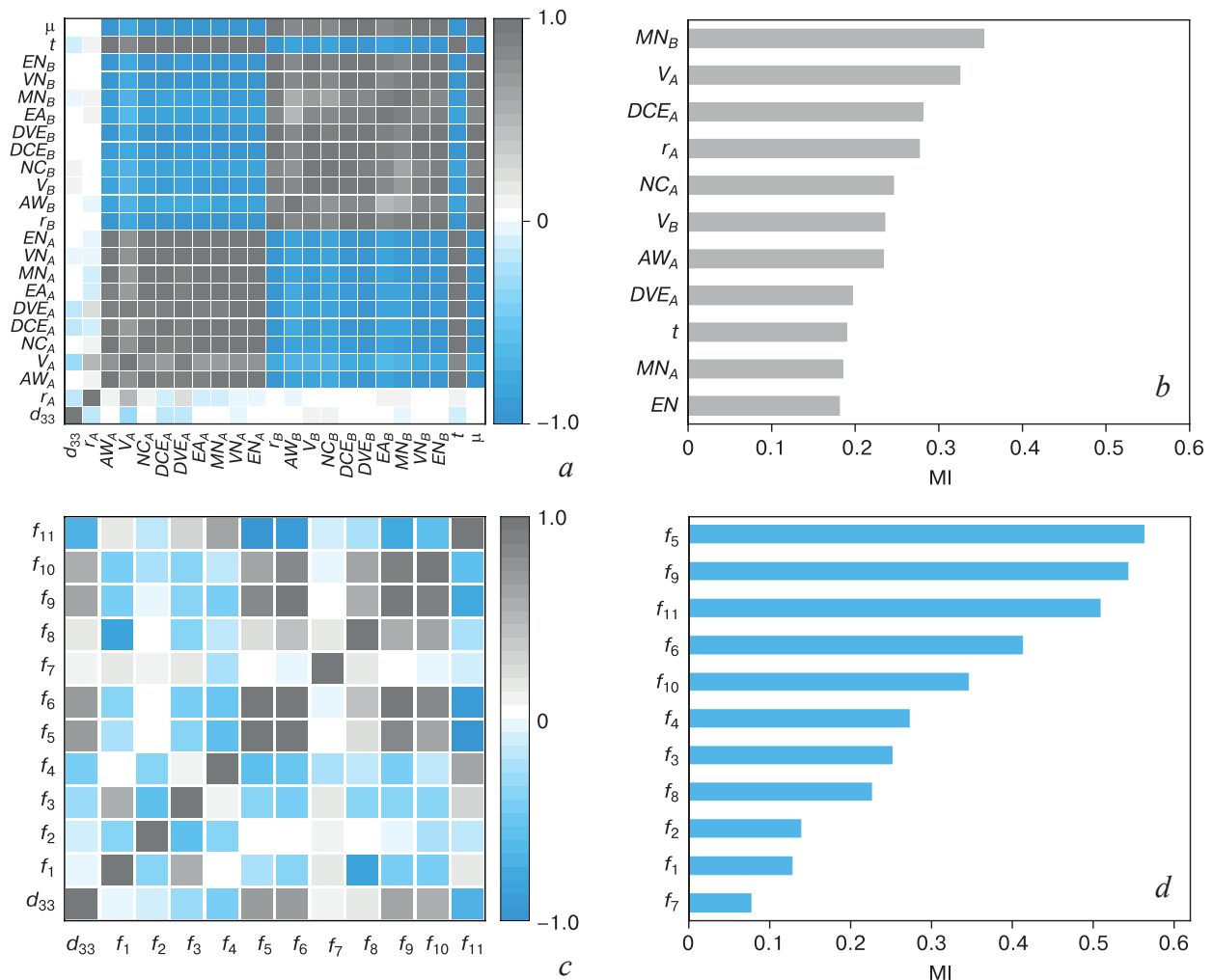


Figure 1. Pearson correlation matrix for (a) initial set of features and (c) SISSO descriptors. Mutual Information for (b) input set of features and (d) SISSO descriptors

The features before and after SISSO application were analyzed using the Pearson heat map and Mutual Information Score (MI) (Fig. 1).

Before SISSO application, the features exhibit a high degree of intercollinearity, the MI value ranging between 0.18 and 0.35. For the SISSO descriptors, the features exhibit a significantly lower degree of mutual correlation, the MI value reaching 0.56. SISSO application reduced the number of features from 22 to 11. Reducing the number of features helps mitigate the risk of overfitting and also lowers the computational cost of both training and prediction.

2.3. Regression machine learning for piezoelectric coefficient

The following machine learning models were learnt using the features f_1 – f_{11} : SVR-linear, Ridge, Lasso, ElasticNet, RF, ETR, GBR, and XGBoost. The models were learnt with 5-fold cross-validation. The predictability of the models was assessed using 80 % of learning data and 20 % of prediction data the learning results are shown in Fig. 2.

The quality of models was assessed by the effective determination coefficient R^2 (Fig. 3), showing the fitness of a model to the initial data set and calculated using the formula

$$R^2 = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y}_i)^2}, \quad (3)$$

where y_i are the actual values, $\hat{y}_i$ are the predicted values, and

$$\bar{y}_i = \frac{1}{n} \sum_{i=1}^n y_i$$

is the average y .

For further analysis, we chose four models with the greatest R^2 and the smallest difference between R^2_{train} and R^2_{test} , showing the stability of the model. The greatest R^2 and smallest $R^2 - R^2_{\text{train}}$ were obtained for the RF, ETR, GBR, and XGBoost models. Those models were then used for the prediction of d_{33} which was measured for KNN samples studies in this work.

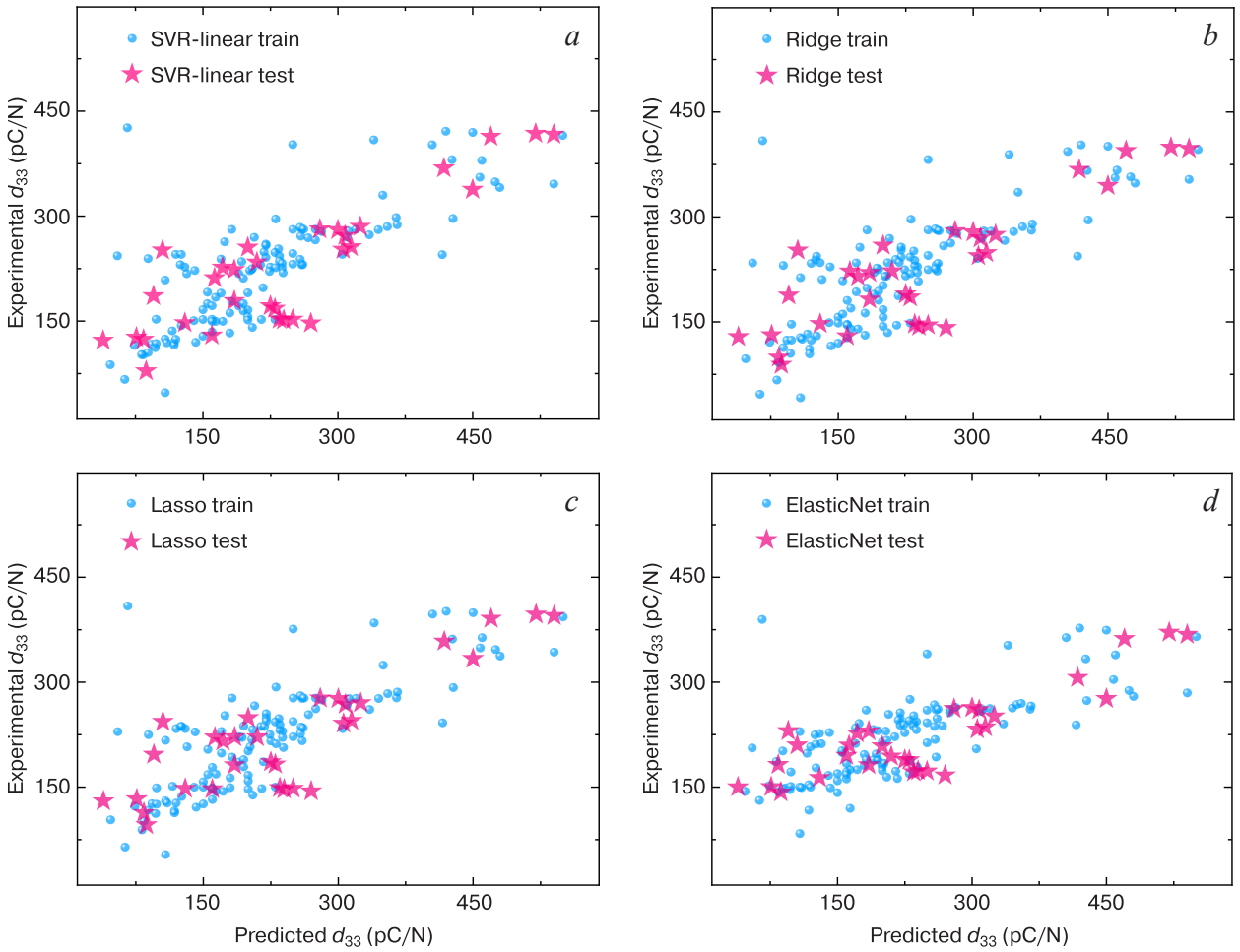


Figure 2. (a–d)

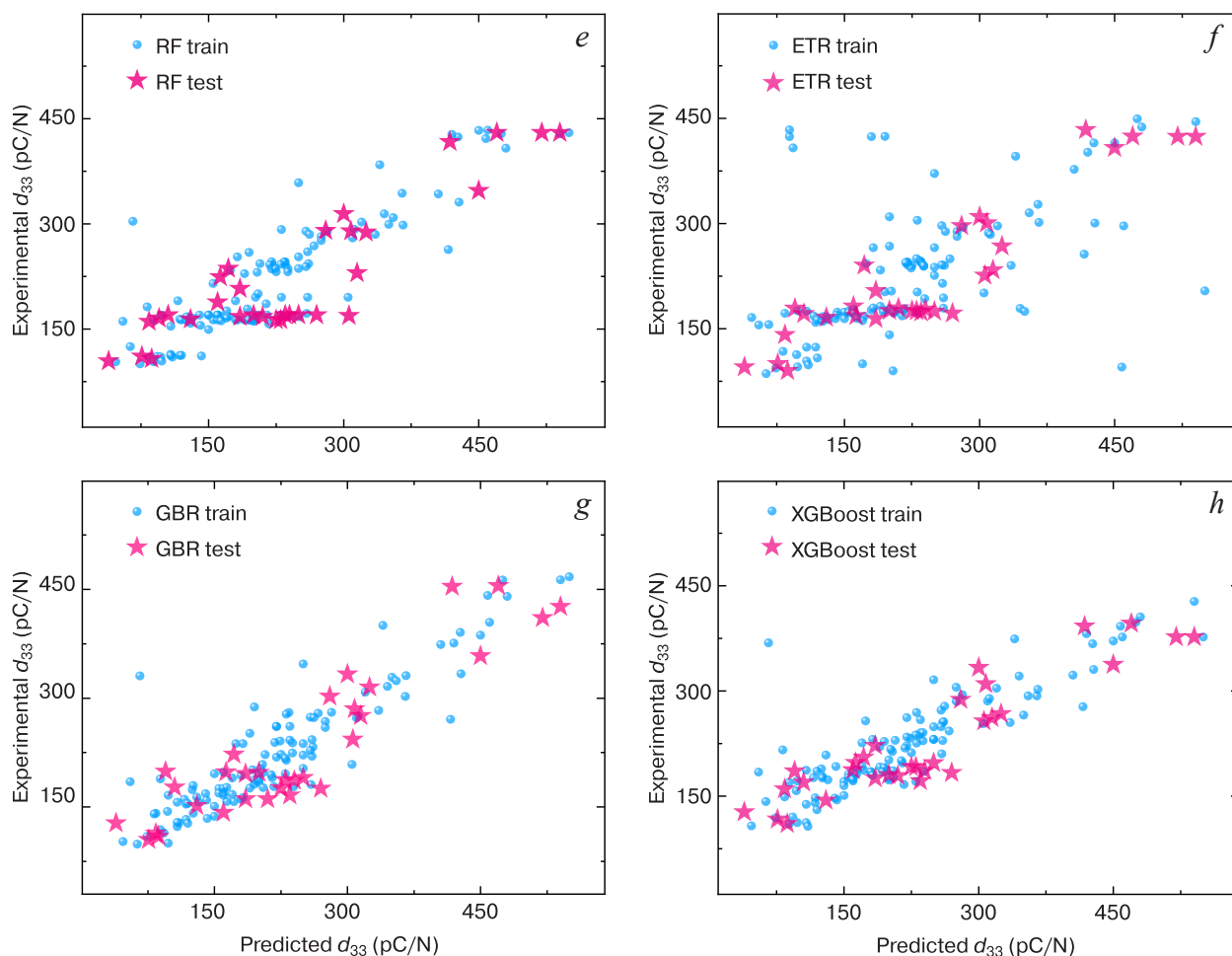


Figure 2. Performance of ML models: (a) SVR, (b) Ridge, (c) Lasso, (d) ElasticNet, (e) RF, (f) ETR, (g) GBR, and (h) XGBoost in prediction of d_{33} for KNN-based ceramics

3. Experimental results

3.1. Samples

The $K_{0.5}Na_{0.5}NbO_3$ sample doped with 1 mol.% barium was obtained by two-stage solid state synthesis. The source reactants were K_2CO_3 , Na_2CO_3 , Nb_2O_5 , and $BaCO_3$. The $KNbO_3$ and $NaNbO_3$ reactants were synthesized at the first stage at 923 and 973 K for 2 h. The as-synthesized $KNbO_3$ and $NaNbO_3$ reactants were crushed, mixed with 1 mol.% $BaCO_3$, compressed to discs 10 mm in diameter and 2 mm in thickness, and sintered at 1373 K for 4 h.

The $(1-x)(K_{0.46}Na_{0.54}Nb_{0.9}Ta_{0.1}O_3) + xLiSbO_3 + 0.02NiO$ samples with $x = 0.02, 0.04$, and 0.06 were obtained by solid state synthesis, the source reactants being $KHCO_3$, $NaHCO_3$, Nb_2O_5 , Ta_2O_5 , Li_2CO_3 , Sb_2O_5 , and NiO . The ceramics were synthesized at 1223 K for 5 h and sintered at 1393 K for 1.5 h.

3.2. Piezoresponse force microscopy

The domain structure and switching and relaxation processes were studied using atomic force microscopy

(NtegraPrima, NT-MDT Spectrum Instruments, Russia) in piezoresponse force microscopy (PFM) mode with NSG10Pt cantilevers (TipsNano). The domain structure of the $0.94(K_{0.46}Na_{0.54}Nb_{0.9}Ta_{0.1}O_3) + 0.06LiSbO_3 + 0.02NiO$ ceramics in the initial state and when exposed

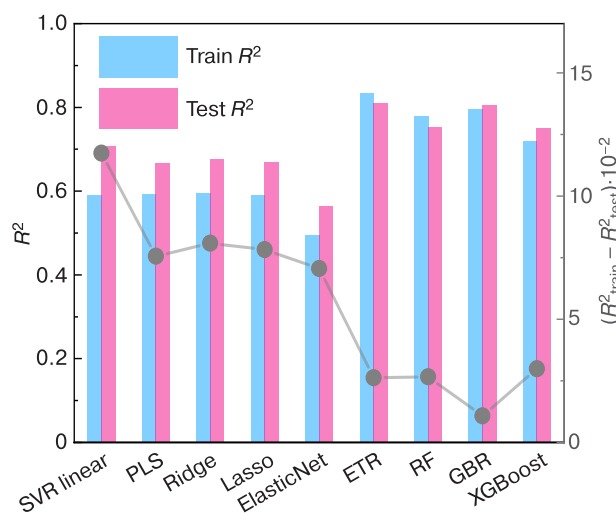


Figure 3. Analysis of ML models performance in prediction of d_{33} for KNN-based ceramics

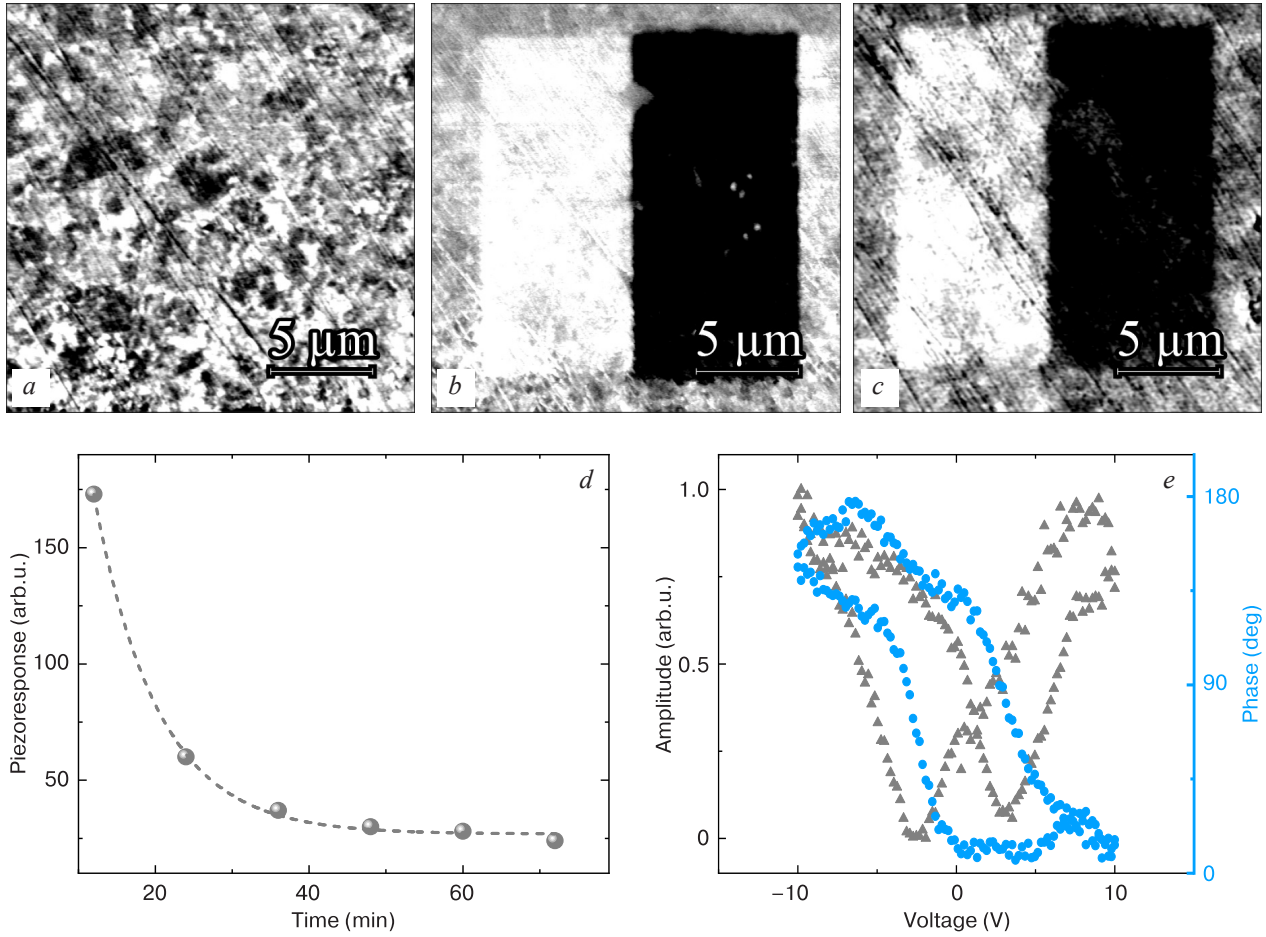


Figure 4. PFM images of (a) initial and induced domain structures in (b) 12 and (c) 72 min after polarization, (d) relaxation curve, and (e) deformation phase and amplitude as a function of voltage

to ± 30 V external electric field are presented in Fig. 4(a–c).

The relaxation curve (Fig. 4d) was measured on the basis of the difference between the piezoresponse signal amplitudes for the positive- and negative-polarized domains. The induced domain structure is stable in time. The off-field deformation phase and amplitude shown in Fig. 4e as a function of voltage confirm the ferroelectric nature of the synthesized ceramics.

3.3. Experimental and prediction d_{33}

For d_{33} measurement, the samples were polarized in an aluminum bath filled with Vaseline oil at 373 K for 2 min in a 24 kV/cm field. The macroscopic piezoelectric coefficient d_{33} was measured using the Berlincur method with a YE2730A d_{33} meter (Sinocera Piezotronics, Inc, China).

The prediction of d_{33} for the KNN ceramics studied in this work was carried out using the following models: RF, ERT, GBR, and XGBoost. The predicted and experimental data are shown in Fig. 5.

The smallest error was demonstrated by the GBR model, the mean absolute error being 26 pC/N.

4. Extracting physical insights from descriptors

The SISSO-obtained descriptors can be divided into the following main groups with respect to the following parameters:

- electronegativity and chemical bond type (f_7);
- Perovskite structure geometry (t , μ) and electronic properties (f_8, f_9, f_{10}, f_{11});
- dimensional parameters and core parameters (f_5, f_6);
- magnetic moment of the B site atom (f_1, f_3, f_4);
- number of valence electrons and distances to the core and valence levels (f_2).

The formulas of the group f_1, f_3, f_4 describe the relationship between the magnetic properties of B site atoms with the volume parameters of A site atoms. It was noted earlier [9] that d_{33} decreases with an increase in the magnetic moment of the B site atom core. The formula f_7 describes the type of chemical bond.

The electron affinity and electronegativity affect the distribution of electron density, which is critical for polarization. It was noted [12] that polarization increases with a decrease in the electronegativity, an increase in the

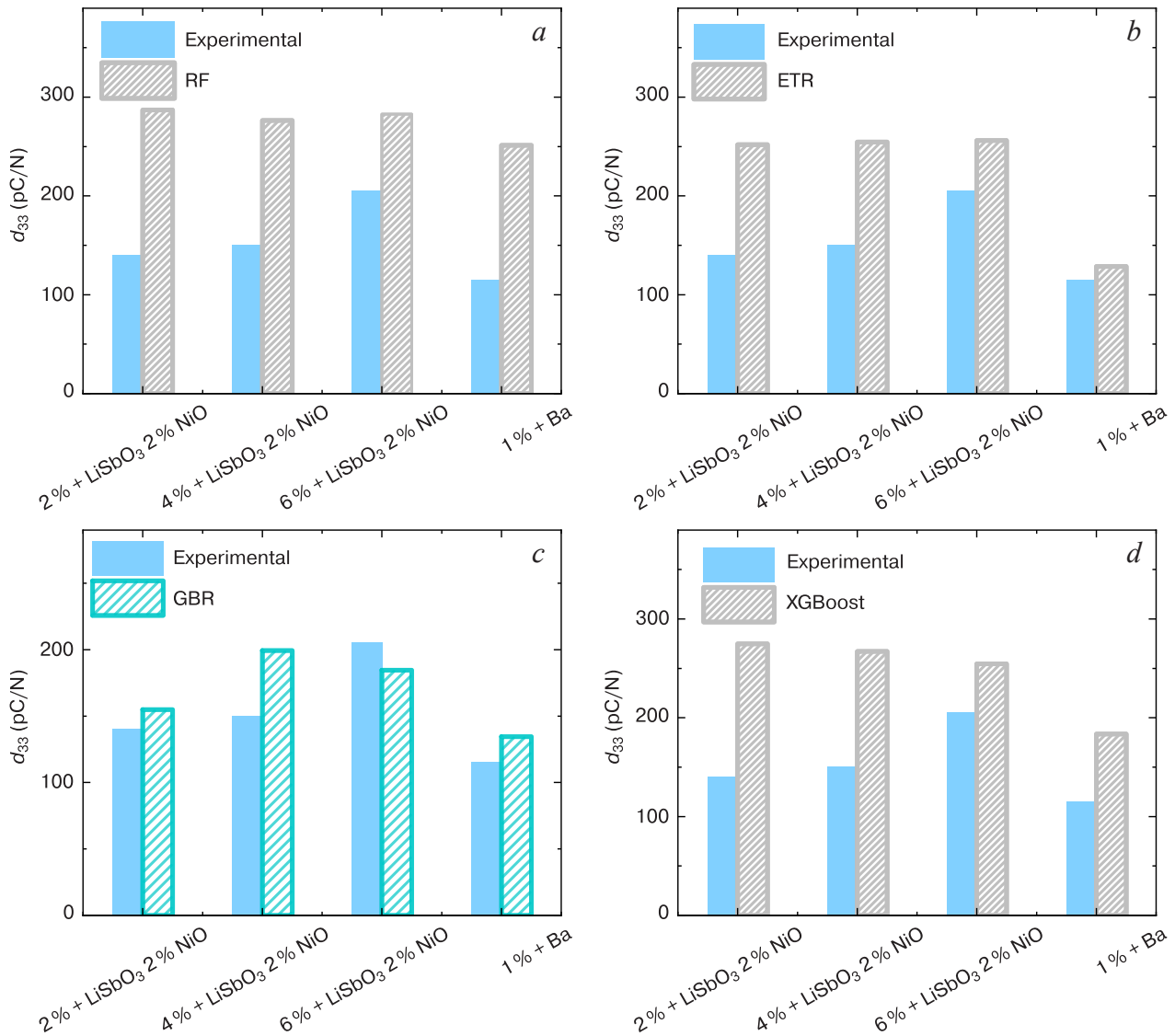


Figure 5. Validation of ML models: (a) RF, (b) ETR, (c) GBR, and (d) XGBoost for independent experimental data

electron affinity and a decrease in the radius of the A site atom.

The descriptors f_5 and f_6 characterize the relationship of the atomic volume and the A site atom nuclear charge with the electron density. The atomic volume affects the deformation of the crystal structure, and high effective nuclear charge can increase atom dilatation.

The descriptors f_8 , f_9 , and f_{11} characterize the relationship between the electronegativity and the geometry of the crystal structure. Electronegativity affects the asymmetry of charge density distribution, favoring the modification of structure geometry, and the emergence of polarization.

Taking into account the earlier calculated MI for SISSO descriptors (see Fig. 1), the descriptors f_5 , f_6 , f_9 , and f_{11} have the greatest significance in the prediction of d_{33} . Thus, the key parameters affecting d_{33} prediction are r_A , V_A , NC_A , NV_A , DCE_A , μ , and t .

Conclusion

The use of the SISSO method allowed identifying the key descriptors for d_{33} prediction: f_5 , f_6 , f_9 , and f_{11} . The key parameters of elements are r_A (effective ionic radii), V_A (volume of atom), NC_A (nuclear charge effective), NV_A (valence electron number), DCE_A (distance from core electron), μ (octahedral factor), and t (Goldschmidt tolerance factor). The GBR method showed the best results in the prediction of the piezoelectricity for the KNN-based ceramics: its accuracy for the test sampling was 81% (the determination coefficient $R^2_{\text{test}} = 0.81$). GBR validation for independent experimental data delivered a mean absolute error of 26 pC/N.

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