

Accelerated design of AgNbO₃-based ceramics with high energy storage performance via machine learning

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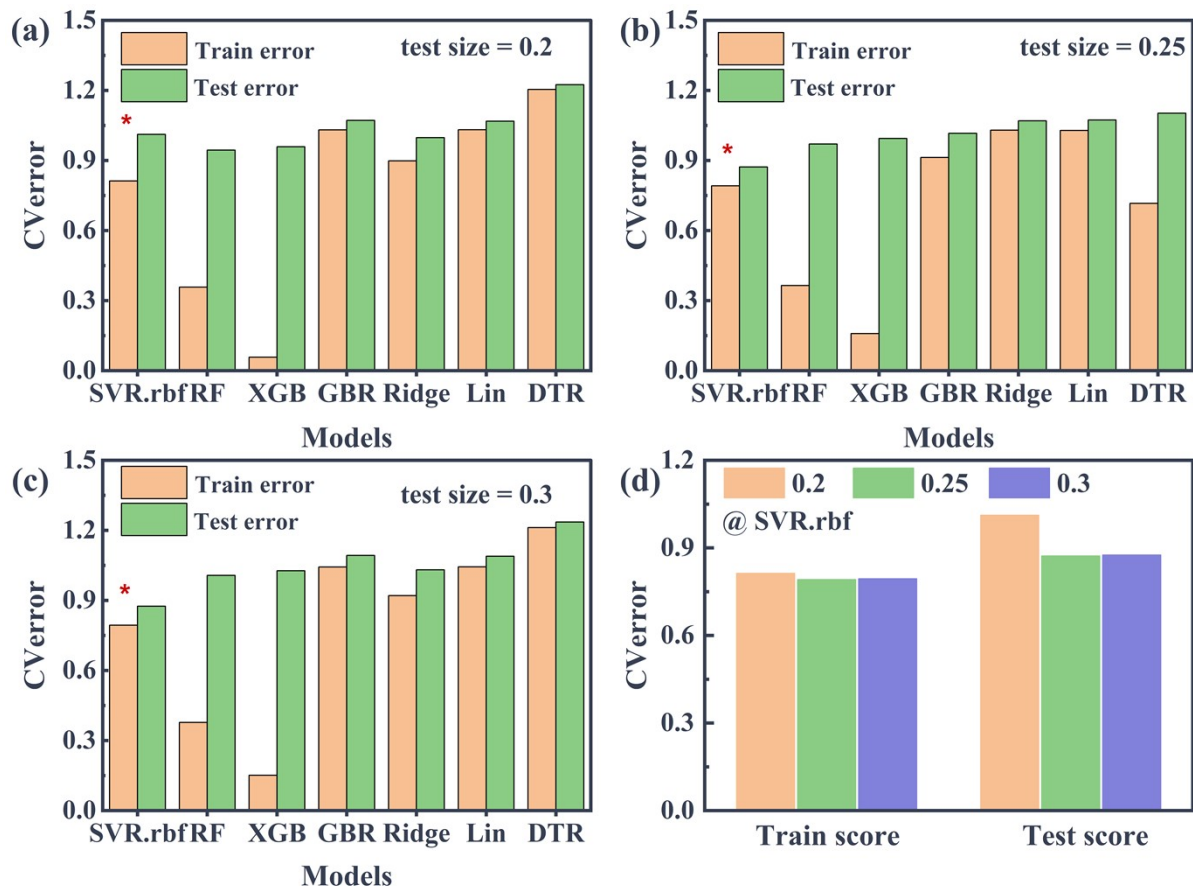


Fig. S1 Model selection using the three descriptors EN-MB, Vec/Z and Rdce with test sizes of (a) 0.2, (b) 0.25, and (c) 0.3. (d) Train error and test error of three test sizes using SVR.rbf model.

To thoroughly assess the predictive performance of the regression model, we split the dataset into three types, namely, 80% for training and 20% for testing, 75% for training and 25% for testing, 70% for training and 30% for testing, as displayed in Fig. S1(a-c). Obviously, the SVR.rbf model exhibits the lowest CVerror on the test observations with adjacent train error and test error for three categories. Moreover, lowest values of both train error and test error are achieved in classification of 75% for training and 25% for testing, as shown in Fig. S1(d).

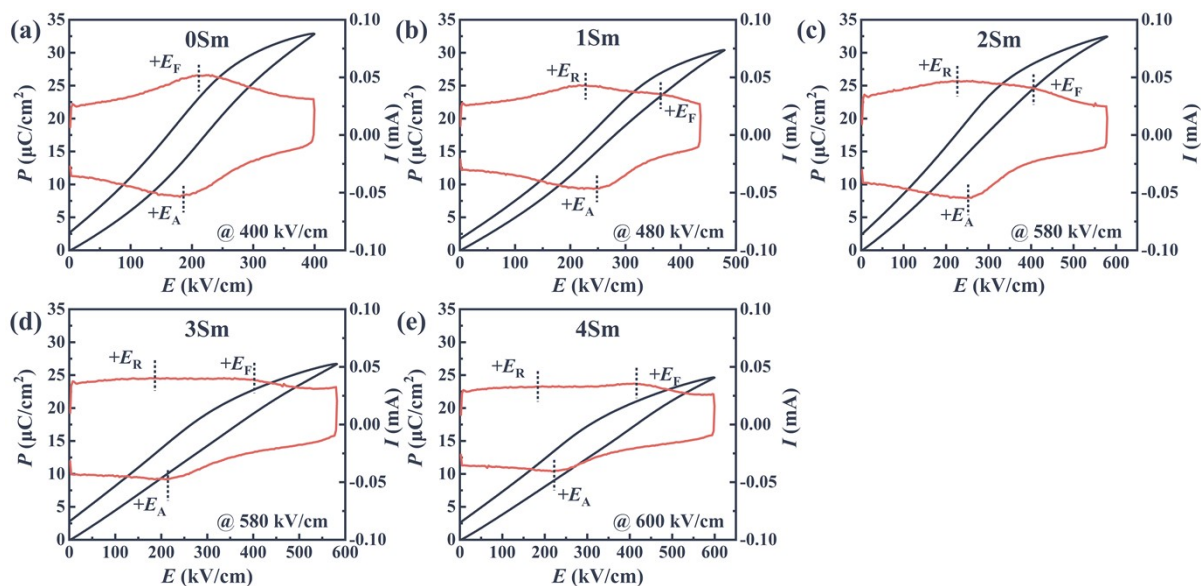


Fig. S2 P - E loops and I - E curves of (a) 0Sm, (b) 1Sm, (c) 2Sm, (d) 3Sm, and (e) 4Sm ceramics at maximum electric field.

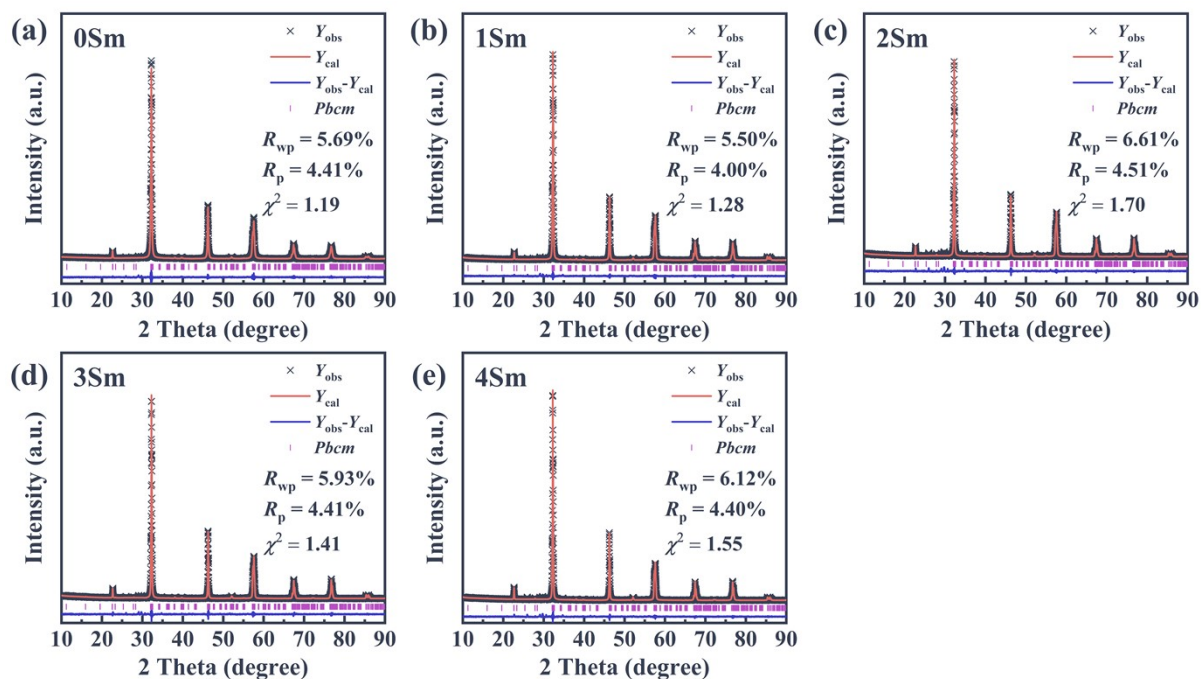


Fig. S3 Rietveld refinement results of (a) 0Sm, (b) 1Sm, (c) 2Sm, (d) 3Sm, and (e) 4Sm ceramics.

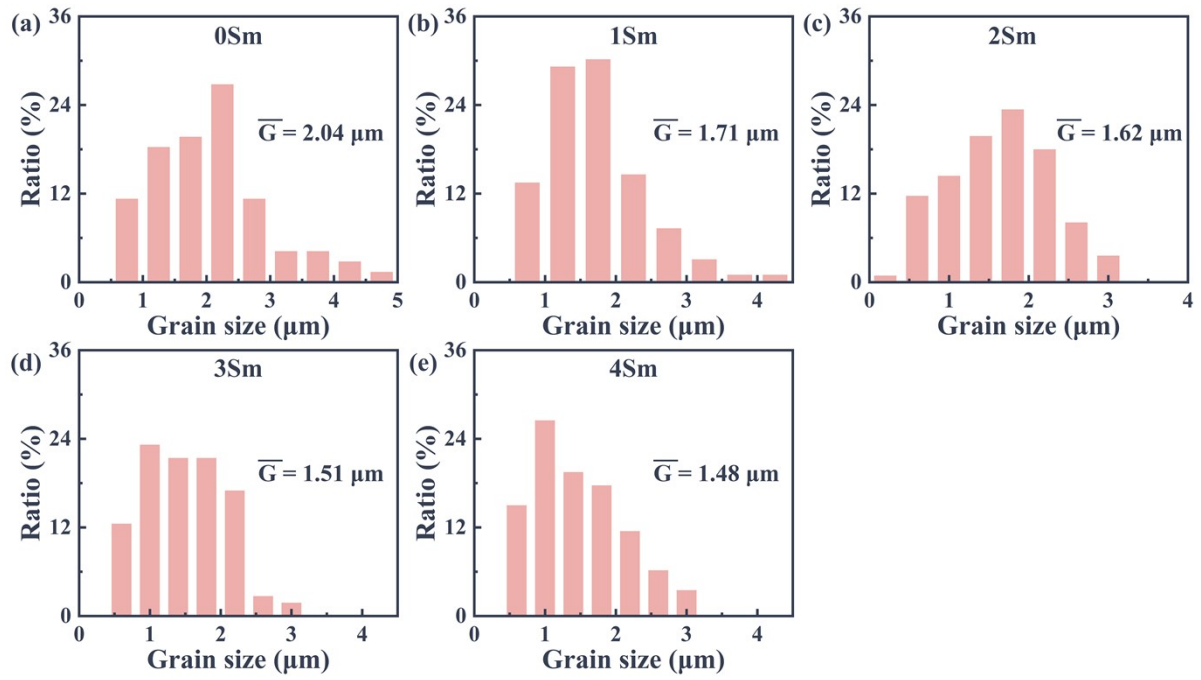


Fig. S4 Grain size distributions of (a) 0Sm, (b) 1Sm, (c) 2Sm, (d) 3Sm, and (e) 4Sm ceramics.

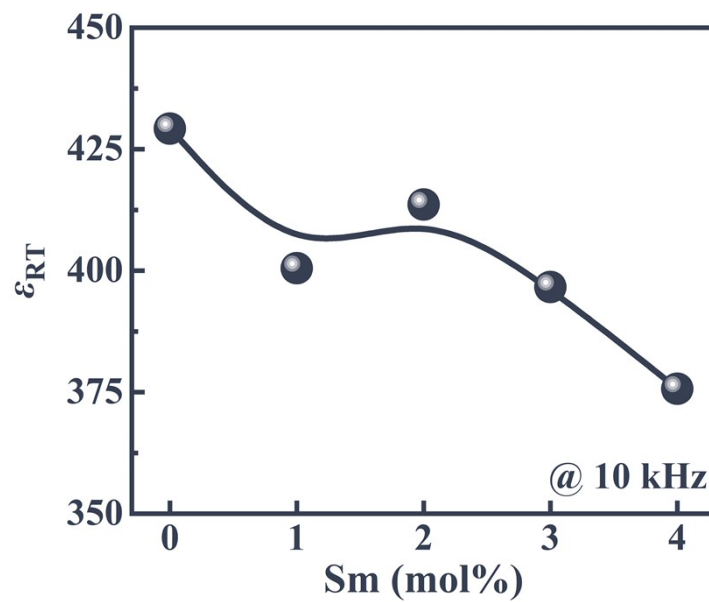


Fig. S5 Room temperature dielectric permittivity for 100xSm ceramics as a function of Sm.