High-throughput screening of ferroelectric materials using support vector machines

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Many researches are going on in the field of high-throughput experimentation (HTE) in the framework of combinatorial catalysis. Some devices that make such HTE possible are developed. However, the rapid progress of those experimental tools requires more diverse data mining methods. In this study, the support vector machine (SVM) is applied to the design of the ferroelectric materials. SVM is a powerful new learning algorithm based on recent advances in statistical learning theory. It generalizes well even though the number of training data sets is small and has been applied successfully to many real world applications. The support vector regression is used to model the relationship between the ferroelectric material compositions (Bi, Ce and La) and the material performances (remanent polarization and coercive field). The proposed model is used to predict the maximum performance, accelerating the discovery of the optimum composition of ferroelectric materials. Acknowledgement