Machine learning extracts structure-stability relationship of substituted Fe-Nd- X structures

*[1]Duong-Nguyen Nguyen, [2]Hiori Kino,[2, 3]Takashi Miyake,[1,2] Hieu-Chi Dam,

[1]Japan Advanced Institute of Science and Technology, Asahidai, Nomi, Ishikawa 923-1292,
[2]Center for Materials Research by Information Integration, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan
[3]CD-FMat, AIST, 1-1-1 Umezono, Tsukuba 305-8568, Japan

We investigate a method for recommending new potential formable Nd-Fe-B crystal structures by using elemental substitution of LA-T-X host structures such as lanthanides (LA), transition metals (T), and light elements (X = B, C, N, O). The 5967 ternary LA-T-X materials are collected from Open Quantum database [1] and used as the host structures. For individual host crystal structure, a substituted crystal structure is created by substituting all lanthanide sites with Nd, all transition metal sites with Fe, and all light element sites with B. High-throughput first-principles calculations are applied to evaluate the phase stability of the newly created crystal structures, and twenty of them are found to be potential formable. An explainable machine learning approach by incorporating supervised and unsupervised learning techniques is applied to analyze the structure–stability relationship of the newly created Nd-Fe-B crystal structures. Three supervised learning models—kernel ridge regression, logistic classification, and decision tree model—learned from the LA-T-X host crystal structures achieve the maximum accuracy and recall scores of 70.4% and 68.7%, respectively, for predicting the stability state of the new substituted Nd-Fe-B crystals. The proposed unsupervised learning model resulting from the integration of descriptor-relevance analysis and a Gaussian mixture model (GMM) provides an accuracy and recall score of 72.9% and 82.1% in predicting the stability of the newly created Nd-Fe-B structures, respectively, which are significantly better than those of the supervised models. In addition, the unsupervised learning model can capture and interpret the structure–stability relationship of the Nd-Fe-B crystal structures. The average atomic coordination number and coordination number of the Fe sites are quantitatively identified as the most important factors in determining the phase stability of the new substituted Nd-Fe-B crystal structures.

References:

[1] Saal, J. E., Kirklin, S., Aykol, M., Meredig, B., and Wolverton, C. "Materials Design and Discovery with HighThroughput Density Functional Theory: The Open Quantum Materials Database (OQMD)", *JOM* **65**, 1501-1509 (2013). doi:10.1007/s11837-013-0755-4