Computational Materials Science

Machine learning-based prediction of phases in high-entropy alloys

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Abstract

“The answer to the question “why HEAs exhibit such exceptional properties” lies in their phases” [1]. The implementation of machine learning (ML) approaches for the classification of solid solution high-entropy alloy (HEA) phases is, therefore, a topical theme in material informatics. For this study, we construct a new dataset based at least 430 peer-reviewed experimental publications including at least 40 metallurgy-specific predictor features. This study proposes a systematic framework incorporating of (a) six feature selection schemes, (b) construction of feature ensembles, and (c) the implementation of eight general ML classifiers. The classifiers, namely: regression tree (DT), linear discriminant analysis (LDA), na ve Bayes (NB), generalized linear regression (GLMNET), random forest (RF), artificial neural networks (NNET), k-nearest neighbors (kNN), and support vector machines (SVM) were trained and evaluated on classifying HEA solid solution phases across feature ensemble sizes. Feature selection results identify the most discriminating predictor features and against intuition, the post-treatment heat-treatment features performed poorly. The RF, SVM, kNN, and NNET classifiers outperformed the other algorithms used with accuracy rates of 97.5%, 95.8%, 94.5%, and 94.0%, respectively. Furthermore, five alloy systems were used to test the validity and applicability of the model - stabilization phases, production of phase transitions, and the triangulation of experimental and ab initio study findings were demonstrated.