The application of theory of evidence in prediction of high-entropy alloys

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Since 2004 a new alloying strategy that combines an equal or high proportion of multi-principal elements to create high-entropy alloys (HEAs), with superior properties such as large strength-to-weight ratios, high tensile strength, as well as corrosion and oxidation resistance, has attracted great attention [1], [2]. To accelerate the HEAs designing process, the modeling of the correlation between the principal element combinations and the high-entropy state of random alloys is essential. So far, only a small number of alloys, among a huge number of potential alloys can be created using this alloying strategy, have been studied [3]. Therefore, the data of known HEAs is not enough to statistically model the correlation of principal element combinations to form a high-entropy alloy. To solve this problem, we propose a model to predict the high-entropy state of random alloys using the theory of evidence. Combination abilities of the multi-principal elements to create high-entropy alloys that extracted from collected data are used as pieces of evidence in the prediction problem of random alloys. In this work, we use a dataset that includes 117 binary alloys as a testbed, the numbers of high-entropy and low-entropy alloys are 60 and 57, respectively. The proposed model is evaluated by comparing to three classification models that are trained by using popular Machine Learning techniques in classification problems such as Support vectors machine (SVM), Logistic regression, and Decision tree. Our work shows better accuracy than the other predictive models in the random alloy classification problem. In addition, the proposed model is applicable to unveil the correlations of multi-principal elements in the high-entropy alloys design process. These extracted correlations can be considered as empirical rules in the HEAs screening process.

References:

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[2] Materials Research Letters, Volume 2, Issue 3:107-123 (2014)
[3] Nature Reviews Materials 4, 515–534(2019)