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Report form of Joint Research Project at ZAIKEN (FY2022)

Title of Project	**Machine learning based prediction of mechanical and physical properties for the development of prolonged service life materials**		
Priority Area	**I-C**		
New proposal			
Name of Main Applicant	**Nguyen Hai Chau**		
Institution	**University of Engineering and Technology, Vietnam National University, Hanoi**	**title**	**Associate Professor**

Aim of the research project

Classical strategies to design new materials are often trial-and-error based and require a large number of experiments and simulations. Thus, the strategies are time consuming and costly. In recent years, new methods, namely machine learning, are combined with orthodox methods in materials science, such as quantum chemical and first principle calculations to speed up and reduce cost of material discovery process, and data of already discovered materials. In this project, we aim to use the machine learning methods to predict mechanical and physical properties such as hardness and yield strength of high-entropy alloys as prolonged service life materials. This research's potential contributions include collecting and enrichment of high-entropy alloys databases with the mentioned properties, and building machine learning prediction models for hardness/yield strength of high-entropy alloys.

Contents and results of the research

In the "Machine learning based prediction of mechanical and physical properties for the development of prolonged service life materials" project, we successfully applied ML techniques to predict mechanical properties [1] and structures of materials including HEAs [2]. Conducting statistical analysis of a HEA's yield strength and phase database [3], we found that there are strong linear relations of derived HEAs yield strength and proportion of added elements [4]. Based on this observation, we proposed a new approach to transform and resample the database, then built an explanable linear model and a prediction model.

The linear model has a modest coefficient of determination (R^2=0.55), but it is better than if it is built on the original database (R^2=0.42). All coefficients of predictors of the linear model (valence electron concentration VEC, electronegativity difference $\Delta\chi$, atomic size difference δ, mixing entropy ΔS_{mix}, and mixing enthalpy ΔH_{mix}) are statistically significant. The model explains that when a HEA H_2 is derived from a HEA H_1, change of yield strength of H_2 with reference to H_1 will be proportional with change of $\Delta\chi$ and ΔS_{mix}, and negatively proportional with change of VEC, δ, and ΔH_{mix} [4].

On the transformed and resampled database, we built a prediction model M_1 using an automatic machine learning framework namely AutoGluon and compared its performance with another prediction model M_2 [5]. M_2 is also built using AutoGluon but on the original database. Comparison shows that cross-validation R^2 of M_1 is 0.85, and that of M_2 is 0.76 [4].

References

1. Ikematsu, K. Utsugi, G. Sato, N. H. Chau, T. Yamamoto, Estimation of the Mechanical Properties of High Entropy Alloys using Machine Learning (poster), 32nd Annual Meeting of the Material Research Society of Japan (MRS-J), 5-7 Dec 2022, Yokohama, Japan.
2. K. Utsugi, M. Kubo, N. H. Chau, M. Brik, T. Yamamoto, Estimation of the geometrical and electronic structures of zircon-type materials using machine learning (poster), 32nd Annual Meeting of the Material Research Society of Japan (MRSJ), 5-7 Dec 2022, Yokohama, Japan.
3. S. Gorsse, et al., Data in brief 21, 2018, 2664-2678.
4. N. H. Chau, G. Sato, K. Utsugi, T. Yamamoto, A new data transformation and resampling approach for prediction of yield strength of high-entropy alloys, submitted to 15th Asian Conference on Intelligent Information and Database Systems (ACIIDS 2023), 24-26 July 2023 Phuket, Thailand.
5. N. Erickson, J. Mueller, A. Shirkov, H. Zhang, P. Larroy, M. Li, A. Smola, AutoGluon-Tabular: Robust and accurate automl for structured data, arXiv, 2020, https://arxiv.org/abs/2003.06505.

Outputs of the project (publications, presentations, patents)

1. Ikematsu, K. Utsugi, G. Sato, N. H. Chau, T. Yamamoto, Estimation of the Mechanical Properties of High Entropy Alloys using Machine Learning (poster), 32nd Annual Meeting of the Material Research Society of Japan (MRS-J), 5-7 Dec 2022, Yokohama, Japan.
2. K. Utsugi, M. Kubo, N. H. Chau, M. Brik, T. Yamamoto, Estimation of the geometrical and electronic structures of zircon-type materials using machine learning (poster), 32nd Annual Meeting of the Material Research Society of Japan (MRSJ), 5-7 Dec 2022, Yokohama, Japan.
3. N. H. Chau, G. Sato, K. Utsugi, T. Yamamoto, A new data transformation and resampling approach for prediction of yield strength of high-entropy alloys, submitted to 15th Asian Conference on Intelligent Information and Database Systems (ACIIDS 2023), 24-26 July 2023 Phuket, Thailand.