

Report form of Joint Research Project at ZAIKEN (FY2021)

Title of Project	Informatics approach for the development of prolonged service life materials		
Priority Area	I-B		
Continuation of joint research in 2020			
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Aim of the research project

Computational simulations such as quantum chemical and first-principles calculations play important roles in design of new materials. Classical strategies to design new materials are often trial-and-error and require a large number of experiments and simulations. Therefore, they are time consuming and costly. In recent years, machine learning techniques are combined with first-principles calculations to speed up and cut down cost of materials design process. In this project, we will continue our results in 2020's "Informatics approach for the development of efficient environmentally conscious materials" project to predict phases of high entropy alloys (HEAs). Prediction of the phases is an important step in materials design process since it helps narrowing down the search space of possible materials thus speed up the design process. Furthermore, properties of HEAs such as hardness and strength and with long service life can be predicted based on their phases. Consequently, we will enrich our HEA databases built in the 2020's project and try to develop new HEAs with demanding properties with the help of such machine learning techniques.

Contents and results of the research

In the “Informatics approach for the development of prolonged service life materials” project, we continued the research of prediction of high-entropy alloy’s phase employing machine learning methods. To increase the accuracy of the phase prediction, we extended our ACIIDS 2021 paper [1] by seeking for additional physical quantities other than valence electron concentration (VEC), atomic size difference, mixing enthalpy, mixing entropy and electronegativity difference. The candidate quantities are average melting temperature, standard deviation of melting temperature, standard deviation of VEC, mean bulk modulus and standard deviation of bulk modulus [2]. Because not all of the elements have experimental bulk modulus (e.g. Sr), bulk modulus related properties are not considered. We conducted a factorial experiment [3] to compare effect of the remaining properties to the accuracy of phase prediction on two high-entropy datasets, namely HEA-118 [4] and MPEA-401 [5]. Statistical analysis of experimental results shows that average melting temperature, standard deviation of melting temperature help increasing prediction accuracy by average 3.34% on HEA-118 and 0.49% on MPEA-401 while standard deviation of VEC does not. We submitted the results to Vietnam Journal of Computer Science [6] as per invitation of ACIIDS 2021 conference committee to selected post-conference publication.

References

- [1] N. H. Chau, M. Kubo, L. V. Hai, T. Yamamoto, Phase Prediction of Multi-principal Element Alloys Using Support Vector Machine and Bayesian Optimization, the 13th Asian Conference on Intelligent Information and Database Systems 2021 (ACIIDS 2021), 7-10 Apr 2021 (online conference <https://aciids.pwr.edu.pl/2021/>).
- [2] S. Y. Lee, S. Byeon, H. S. Kim, H. Jin and S. Lee, Deep learning-based phase prediction of high-entropy alloys Optimization, generation, and explanation, Materials and Design 197 (2021) p. 109260
- [3] J. Lawson, Design and analysis of experiments with R, Chapman and Hall/CRC Press, 2014.
- [4] N. Islam, W. Huang and H. Zhuang, Machine learning for phase selection in multi-principal element alloys, Computational Materials Science, vol. 150, pp. 230-235, 2018.
- [5] Huang, W., Martin, P., Zhuang, H.L.: Machine-learning phase prediction of high-entropy alloys. Acta Materialia 169, 225–236 (2019).
- [6] N. H. Chau, M. Kubo, L. V. Hai, T. Yamamoto, Support Vector Machine-based Phase Prediction of Multi-principal Element Alloys, submitted to Vietnam Journal of Computer Science (ISSN (print): 2196-8888 | ISSN (online): 2196-8896).

Outputs of the project (publications, presentations, patents)

N. H. Chau, M. Kubo, L. V. Hai, T. Yamamoto, Support Vector Machine-based Phase Prediction of Multi-principal Element Alloys, submitted in 2022 to Vietnam Journal of Computer Science (ISSN (print): 2196-8888 | ISSN (online): 2196-8896).