Project No. 02413

Report form of Joint Research Project at ZAIKEN (FY2024)

Title of Project	Data analysis and machine learning based prediction of mechanical and physical properties for the development of energy saving materials		
Priority Area	I-B(Prolongation of service life & Structures), I-C(Prolongation of service life & Properties), III-B(Energy saving & Structures), III-C(Energy saving & Properties)		
Continuation of FY2023 project			
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

In recent years, machine learning (ML) has been increasingly integrated with traditional methods in materials science, such as quantum chemistry and first-principles calculations, to accelerate and reduce the cost of the material discovery process. One of the most prevalent applications of ML in materials science is the prediction of novel materials with desired properties. However, most ML methods typically offer point predictions, meaning single continuous (e.g., yield strength) or discrete (e.g., phase) values. Prediction regions such as intervals or sets of discrete values are often unavailable, leaving the uncertainty of predictions unknown. Our primary objective in this project is to quantify the uncertainty of machine learning prediction models for properties of high-entropy alloys (HEAs) including Young's modulus and yield strength. This research aims to contribute by enriching and analyzing HEA databases and quantifying prediction regions for ML prediction models of these properties. Quantifying prediction regions is crucial for determining which predictions warrant experimental validation.

Contents and results of the research

High-entropy alloys (HEAs) are materials typically composed of five or more principal elements, each with an atomic concentration usually ranging between 5% and 35%. Recently, HEAs have gained significant research attention due to their superior mechanical and physical properties, such as yield strength and hardness, compared to conventional alloys [1, 2]. There are three main approaches for designing new materials, including HEAs: density functional theory (DFT), high-throughput (HT), and machine learning (ML). ML leverages both experimental data and data generated from DFT and HT methods to predict the properties and structures of new materials [3, 4, 5].

ML is increasingly integrated with established methods in materials science, such as quantum chemistry and first-principles calculations, to accelerate and reduce the cost of material discovery. While ML excels at predicting material properties, it primarily captures correlations rather than causal relationships, limiting its ability to explain cause-and-effect mechanisms [6]. While causal studies in materials science exist, they are typically case-specific [7, 8, 9, 10]. Although these studies provide valuable experimental data and insights into specific causal relationships, their findings may not be generalizable to other cases.

In this project, we have developed a novel causal model, the High-Entropy Alloy Causal Model (HEACM), for the first time to estimate the effects of key variables—specifically valence electron concentration (VEC), mixing enthalpy (ΔHmix), and mixing entropy (ΔSmix)—on the yield strength (YS) of HEAs [11]. Unlike traditional machine learning models that primarily capture correlations, HEACM aims to uncover cause-and-effect relationships, enabling a more interpretable understanding of material properties. Our experimental results show that when varying the atomic concentration of a single element in HEA compositions, an increase of one unit in VEC or ΔHmix results in a decrease in YS, with an average reduction of 252.3 MPa and 29.8 MPa, respectively. Conversely, an increase of one unit in ΔSmix leads to an increase in YS by an average of 217.4 MPa. These findings highlight the potential of HEACM as a practical approach for designing high-performance HEAs, particularly when combined with machine learning approaches to enhance both causality and predictability.

References

1. D. B. Miracle, O. N. Senkov, Acta Mater. 122, 2017, 448-511.
2. Y.F. Ye, et al., Mater. Today 19(6), 2016, 349-362.
3. G. R. Schleder, et al., J. Phys.: Condens.Mater. 2, 2019, 032001.
4. C. K. H. Borg, et. al., Sci Data 7, 2020, 430.
5. S. Gorsse, et al., Data in brief 21, 2018, 2664-2678.
6. S. Arif, M.A. MacNeil, Predictive models aren't for causal inference, Ecology Letters 25 (2022).
7. J. Kumar, A. Linda, M. Sadhasivam, K.G. Pradeep, N.P. Gurao, K. Biswas, The effect of Al addition on solid solution strengthening in CoCrFeMnNi: Experiment and modelling, Acta Materialia 238 (2022).
8. Y. Chen, W. Liu, H. Wang, J. Xie, T. Zhang, L. Yin, Y. Huang, Effect of Ti content on the microstructure and properties of CoCrFeNiMnTix high entropy alloy, Entropy 24 (2022).
9. Z. Feng, C. Zhang, C. Gu, M. Xu, L. Yang, L. Wang, J. Yi, Effect of Ti on microstructure and mechanical properties of CoFeNiVTix high-entropy alloys, Journal of Materials Engineering and Performance (2023)
10. S. Chen, L. Bao, H. Yang, X. Si, Q. Yu, Effect of Al content on microstructure and mechanical properties of Alx(Nb3TaTi3Zr)100-x refractory high-entropy alloys, Journal of Physics: Conference Series 2691, 12071 (2024).
11. N. H. Chau and T. Yamamoto, "Effects of changing atomic concentration of a single element on the yield strength of high-entropy alloys: A causal inference study," Journal of Electronic Materials, pp. 1–12, 2025. Topical collection: Frontiers in Materials Science 2024.

Outputs of the project (publications, presentations, patents)

1. N. H. Chau and T. Yamamoto, "Effects of changing atomic concentration of a single element on the yield strength of high-entropy alloys: A causal inference study," Journal of Electronic Materials, pp. 1–12, 2025. Topical collection: Frontiers in Materials Science 2024.