Project No. 02511

Report form of Joint Research Project at ZAIKEN (FY2025)

Title of Project	**Causal Inference for Investigating Property-Structure Relationships in High-Entropy Alloys and Energy-Efficient Materials**		
Priority Area	**I-B, I-C, III-B, III-C**		
New proposal or **Continuation of**			
Name of Main Applicant	**Nguyen Hai Chau**		
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Aim of the research project

Machine learning (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. Existing causal studies in materials science are often case-specific and lack generalizability.

This project aims to estimate the causal effects of varying atomic concentrations of multiple elements—such as in high-entropy alloys (HEAs) and optical materials—on their desired properties. By leveraging key variables like electronegativity, mixing enthalpy, and mixing entropy, we seek to answer: How much does a desired property change when a key variable shifts by one unit? Using causal inference (CI), our findings will provide deeper insights into materials development by uncovering fundamental causal relationships.

Contents and results of the research

(Please indicate to which extent the expected objectives in your proposal have been achieved.)

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%. 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]. Researchers usually use Density Functional Theory (DFT), high-throughput (HT), Machine Learning (ML), or combination approaches to design them. While ML is good at predicting properties, it only based on correlations. It does not explain the actual cause and effect [3]. Most causal studies today are also limited to specific cases and are hard to apply generally [4, 5, 6, 7].

In 2025, we focused our project on the hardness of HEAs. We developed a new version of the HEACM model [8] called HEACM for hardness [9]. This model uses Double/Debiased Machine Learning (DoubleML) [10] to find the causal impacts of the key variables: valence electron concentration (VEC), mixing enthalpy (ΔHmix), and mixing entropy (ΔSmix) on the hardness of HEAs. Our new results show how these variables change the hardness of HEAs:

- A one-unit increase in valence electron concentration (VEC) leads to a decrease in Vickers hardness by 184.29 units (robustness value = 31.7%).
- A one-unit increase in mixing enthalpy (ΔHmix) leads to a decrease in Vickers hardness by 3.38 units (robustness value = 8.35%).
- A one-unit increase in mixing entropy (ΔSmix) leads to an increase in Vickers hardness by 44.37 units (robustness value = 21.3%).

Future research direction: We now have two causal models: the HEACM model for yield strength [8] and the new model for hardness [9]. Our next step is to develop a causal framework for the trade-offs between hardness, strength, and ductility - a classic and critical problem in HEA research.

References

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9. T. K. Ly, N. H. Chau, and T. Yamamoto, "A causal inference approach to assess the effects of atomic concentration changes on the hardness of high-entropy alloys," in Computational Collective Intelligence (N. T. Nguyen, V. Dinh Duc Anh, A. Kozierkiewicz, S. Nguyen Van, M. Núñez, J. Treur, and G. Vossen, eds.), (Cham), pp. 152–166, Springer Nature Switzerland, 2026.
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Outputs of the project (publications, presentations, patents)

1. T. K. Ly, N. H. Chau, and T. Yamamoto, "A causal inference approach to assess the effects of atomic concentration changes on the hardness of high-entropy alloys," in Computational Collective Intelligence (N. T. Nguyen, V. Dinh Duc Anh, A. Kozierkiewicz, S. Nguyen Van, M. Núñez, J. Treur, and G. Vossen, eds.), (Cham), pp. 152–166, Springer Nature Switzerland, 2026.