VIDEO ARTICLE

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Combining CALPHAD and Machine Learning to Design Single-phase High Entropy Alloys

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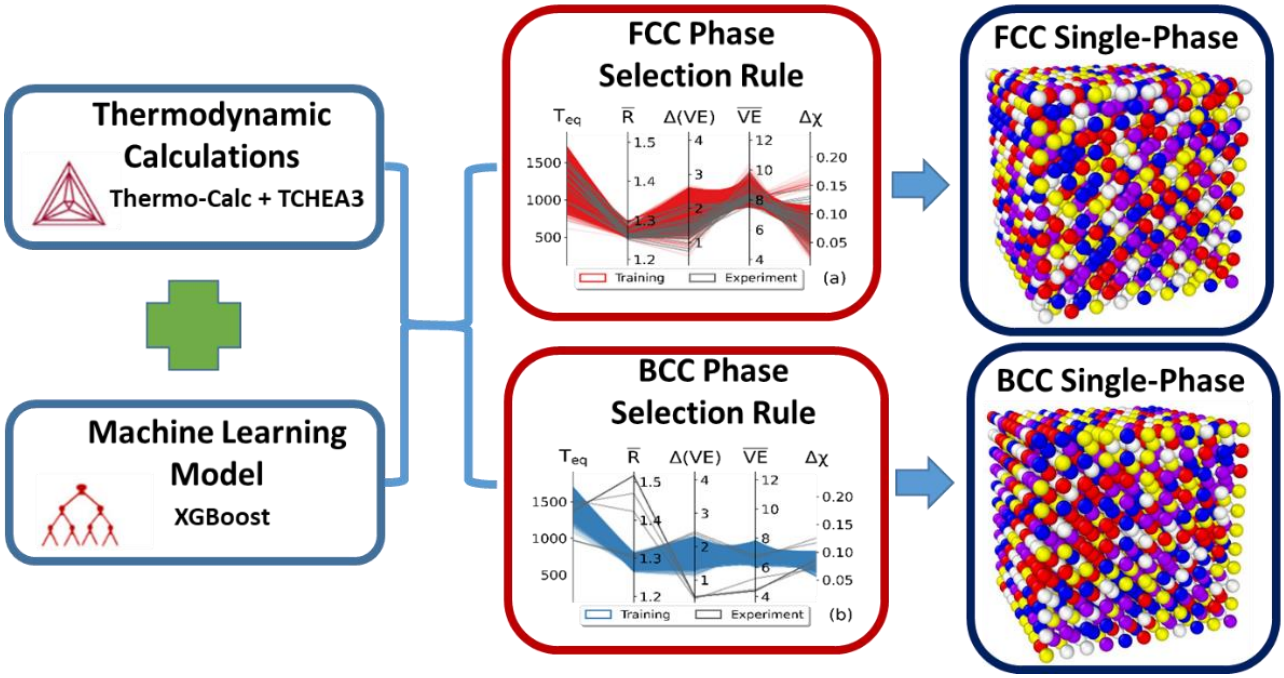
Graphical Abstract



By combining CALPHAD and machine learning to develop phase selection rules, and further to design single-phase HEAs.

Abstract

Although extensive experiments and computations have been performed for many years, the phase selection rules and prediction of single-phase HEAs currently remain elusive [**1**]. An underlying reason is that many of these phase selection rules were proposed or developed based on experimental data of limited composition spaces and/or insufficient data, and thus they are often not robust for the phase selection of HEAs. Machine learning (ML) methods have recently been used to predict the phase formations/selections of HEAs and achieved a certain degree of success. However, they still suffer the problems of small datasets and irrational selection of suitable physical descriptors. Moreover, ML

models are often perceived as a 'black box' to the materials research community, thus often lack of clear physical meaning/understanding [**2**]. To effectively guide the design of HEAs, it is important and necessary to develop convenient and yet effective phase selection rules. In the talk, we report our research work on combining CALPHAD machine learn to design single-phase high entropy alloys. First, we used Thermo-Cal software together with the database TCHEA3 to generate a large dataset with more than 300,000 quinary data formed by Al, Co, Cr, Cu, Fe, Mn, Ni, and Ti. Next, we selected initial 15 features and employed a machine learning model to rank their importance. Based on the ranking, we then further performed feature reduction and identified most important features that governed the formation of single phases of FCC, BCC and other phases. Our study showed that at least 5 important features were needed to best discriminate the three classes of phases. These 5 features are equilibrium temperature, average atomic radius, average valence electron, difference in electronegativity, and difference in valence electron. The inclusion of equilibrium temperature, which was often neglected in previous studies, highlights its importance in the phase selection of HEAs. Our ML model was tested on 155 experimental data and reached a high accuracy of 81%. Based on the 5 important features and the large dataset, we established new phase selection rules for HEAs of single-phase FCC and BCC and achieved the accuracy of 93% and 92%, respectively. In addition, we also clarified the controversy concerning the phase selection rules in HEAs and offered in-depth insights into the relationships among composition-feature-phase of HEAs. Finally, we designed 222 new single-phases HEAs of BCC and FCC structures for experimental exploration [**3**].

Keywords: High entropy alloy, CALPHAD, Machine learning; Phase selection rule.

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Biography of Presenting Author

Yong-Wei Zhang is Principal Scientist II and Deputy Executive Director (Research) at Institute of High-Performance Computing, A*STAR, Singapore. He received his Ph.D from Northwestern Polytechnical University, Xi'an, China. Subsequently, he worked at Institute of Mechanics, Chinese Academy of Sciences, China; School of Engineering, Brown University, USA; Institute of Materials Research and Engineering, Singapore; and National University of Singapore. Currently, he is also an Adjunct Professor at National University of Singapore and Singapore University of Technology and Design. His research interests focus on developing/using theory, modelling and simulation to investigate the structural, mechanical, electronic, thermal and chemical properties of materials for new material design, additive manufacturing, micro- and nano-electronics, energy

conversion and storage et al. He has published about 500 peer reviewed international journal papers with total citations of > 27,000 and h-index of 79 (based on Google Scholar). He also delivered more than 80 invited/keynote/plenary talks and lectures at many prestigious international conferences and institutions. He has been listed as Global Highly Cited Researchers in 2018, 2019 and 2020 by Web of Science Group. He is a Vebleo Fellow and a winner of IPS World Scientific Physics Research Medal and Prize. He also serves as an Editorial Board Member for Advanced Theory and Simulation (Wiley), Modelling and Simulation in Materials Science and Engineering (IOP), International Journal of Applied Mechanics (World Scientific), and Acta Mechanica Sinica (Springer).

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