Webinar-38
Asian Consortium on Computational Materials Science (ACCMS) Centre
SRM University-AP, Amaravati, Andhra Pradesh, India

Title: Exploring Transition Metal High Entropy Alloys from First-principles and Machine Learning

Abstract

This research series was started from two quinary HEAs, Cantor alloy FeCoNiCrMn, and FeNiCoCrPd, which were synthesized by intentionally substituting Mn in Cantor alloy with Pd, and this new HEA was reported to be achieved at 2.5 times higher strength than Cantor alloy. We investigated the stability and structural properties of these two HEAs based on first-principles calculation combing finite temperature effects using the special quasi-random structures (SQS) as model of solid solution. It has been revealed that the inhomogeneous introduced by Pd consequences the enhancement of the mechanical properties. The study has been extended to 6-element HEA with introducing Al into FeCoNiCrMn/Pd and it is found that the partial ordering relates very much to the fcc-bcc transformation with varying Al concentration. Along this work, more than 1,000 DFT SQS data have been accumulated, including all sub-systems of binary, ternary, quaternary in all equiatomic compositions and typical non-equiatomic compositions of FeCoNiCrMn/Pd, for fcc, bcc and hcp structures. Based on this data set, systematic predictions are conducted by machine learning. Using the elemental convolution graph neural networks (ECNet) in cooperating with transfer learning, three new compositions of $(FeCoNiCrMn)_{1-x}Pd_x$ with superior mechanical property to known HEAs have been discovered. To further explore new compositions with excellent properties in a wide searching space from limited first-principles calculation data, we attempted the data augmentation technology using both the generative AI (GAN) and the physical method of cluster expansion (CE). These results enriched the physics of high entropy alloys.

PROF. YING CHEN
Professor
Tohoku University

Panelist

DR. SHEN LEI
Senior Lecturer,
National University of Singapore

Short Biography

Ying Chen, Professor at Tohoku University, Japan, majored in solid state physics. The main research field is computational materials science based on first principles, combining materials informatics. She has been actively involved in several large Japanese national research projects to conduct computational research on a wide range of materials such as intermetallics, alloys, steel, nuclear materials, permanent magnets, and high entropy alloys. Ying Chen received her Master's degree from the University of Science and Technology Beijing, PhD from the University of Tokyo in 1996. After working in the Japan Science and Technology Agency (JST) for six years, she became an Associate Professor in the School of Engineering, the University of Tokyo in 2002, moved to Tohoku University in 2009, and was promoted to a full Professor of the School of Engineering of Tohoku University in 2013. She was appointed as a Professor at the Global Learning Center of Tohoku University in April 2025. Ying Chen is a member of the Engineering Academy of Japan (EAJ).

Conveners:

Prof. Yoshiyuki Kawazoe, Head, ACCMS-Centre
Prof. G P Das, TCG Crest
Prof. Ranjit Thapa, SRM University-*AP*

Local Organisers:

Dr Mahesh Kumar Ravva, SRM University–*AP*
Prof. Umesh Waghmare, JNCASR
Dr Surya VJ, ACCMS

Zoom Meeting Link

https://srmap.zoom.us/j/95035900331?
pwd=ahqfYjobEEBrlBNdrTEZPh7vc12gqx.1
Meeting ID: 950 3590 0331
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📅 **November 25, 2025**

🕐 **01:00 PM - 02:30 PM IST**

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