VIDEO ARTICLE

Vid. Proc. Adv. Mater., Volume 3, Article ID 2210360 **(2022)**

Alloy Design in the Information Age and Beyond

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DOI: 10.5185/vpoam.2022.10360

Abstract

Alloy discovery has been greatly accelerated by techniques of artificial intelligence in the modern Information Age. In this talk, I will use a new family of alloys called high-entropy alloys (HEAs) as an example to demonstrate how state-of-the-art machine learning algorithms are applied to discover new HEAs that exhibit excellent properties that largely depend on the selection among three phases: solid solution (SS), intermetallic compound (IM), and mixed SS and IM (SS+IM). Accurate phase prediction is therefore crucial for guiding the selection of a combination of elements to form a HEA with desirable properties. The phase selection is correlated with elemental features such as valence electron concentration and the formation enthalpy, leading to a set of parametric phase-selection rules. Here we employ machine learning algorithms to efficiently explore phase selection rules using a comprehensive experimental dataset consisting of 401 different HEAs including 174 SS, 54 IM, and 173 SS+IM phases. We adopt three different machine learning algorithms: K-nearest neighbors, support vector machine, and artificial neural network. Our work provides an alternative route of computational design of HEAs, which is also applicable to accelerate the discovery of other metal alloys for modern engineering applications.

References

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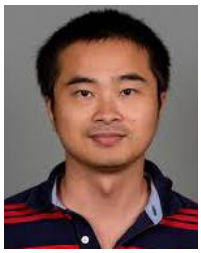
Biography of Presenting Author



Houlong Zhuang is currently an Assistant Professor in the School for Engineering of Matter, Transport and Energy at Arizona State University. He obtained his doctorate in Materials Science and Engineering at Cornell University in 2014. He worked as a postdoctoral researcher at Oak Ridge National Laboratory from 2014-2015, and as a postdoctoral fellow at Princeton University from 2015-2017. He was trained as a theoretical and computational materials scientist in various fields of materials science and engineering, especially in energy-related areas including catalysis, lightweight metal alloys, two-dimensional materials, and solid/liquid interfaces. His current research is focused on applying quantum mechanical simulations, machine learning, and quantum computing calculations to tackle issues such as hydrogen storage and direct air capture for a sustainable energy and environment future. Dr. Zhuang is a recipient of the 2022 Materials Today Rising Star Award. He is a Scialog Fellow for Negative Emissions Science and a Fellow of the International Association of Advanced Materials.

Citation of Video Article

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