Contribution ID: **50** Type: **Talk**

Design of high-entropy Invar alloys via machine learning (12 min talk + 3 min discussion)

Wednesday, 14 April 2021 14:45 (15 minutes)

Invar alloys exhibit a very low thermal expansion coefficient (TEC) below 2×10−6 K−1 around room temperature. There is a strong impetus to design novel Invar alloys with better physical, mechanical and chemical properties. Here, we develop and apply an active learning strategy to accelerate the design of novel Invar alloys in a practically infinite compositional space of quaternary and quinary high-entropy alloys (HEAs).It is demonstrated that this strategy is of great potential to accelerate the discovery of novel functional materials, especially for those with large unexplored phase space such as compositions, crystal structures, and microstructures.

Poster title

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Session Classification: Session I