Theory-guided Design of High-strength, Ductile, Single-phase BCC High Entropy Alloys

Y. Rao[1], C. Baruffi[1], A. De Luca[2], C. Leinenbach[2] and W.A. Curtin[1]

[1]*Laboratory for Multiscale Mechanics Modeling, EPFL, 1015 Lausanne, Switzerland*

[2]*Empa – Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland*

The immense compositional space of High Entropy Alloys (HEAs) presents possibilities of discovering compositions that satisfy various application requirements. We introduce a theory-based and parameter-free materials selection procedure that takes into account both mechanical and thermodynamic properties of the target alloys. We first make selections of single phase equiatomic quinary BCC refractory HEAs that are both strong and ductile at room temperatures. Not limited to certain compositions, the procedure is also used to search the off-equiatomic domain to further tailor alloy properties to specific needs, where we have found 10 quinaries and 15 quaternaries that have lower densities but comparable or even higher specific strength than their equiatomic counterparts. To validate the selection procedure, we have fabricated and characterized one of the alloys. The experiment results agree well with our prediction. This procedure provides a reliable way to quickly pinpoint target alloys, greatly facilitating the discovery of next generation materials.