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High entropy alloys: mechanical properties and phase stability

The term “High entropy” alloys (HEA) refers to a relatively new class of multicomponent—usually five or more—metallic alloys in equal or near equal atomic concentrations. Instead of ordered intermetallics, expected from classical physical metallurgy, some HEA systems strikingly crystalize as single phase solid solutions with simple crystal structures. The complex compositions of these alloys, and their derivatives, lead to unique properties. They also encourage new ways of viewing fundamentals of physical metallurgy, yielding new insights that are applicable to a wide range of metallic alloys. In this talk I will present two aspects of these systems: mechanical properties and thermodynamics.

In the first part, I present a phase transformation strengthening mechanism in CrCoNi, a ternary derivative of the CrMnFeCoNi high entropy alloy. CrCoNi alloy exhibits a remarkable combination of strength and plastic deformation, even superior to the CrMnFeCoNi high-entropy alloy. We connect the magnetic and mechanical properties of CrCoNi, via a magnetically tunable phase transformation. While both alloys crystallize as single-phase face-centered-cubic (fcc) solid solutions, we find a distinctly lower-energy phase in CrCoNi alloy with a hexagonal close-packed (hcp) structure. Comparing the magnetic configurations of CrCoNi with those of other equiatomic ternary derivatives of CrMnFeCoNi confirms that magnetically frustrated Mn eliminates the fcchcp energy difference. This highlights the unique combination of chemistry and magnetic properties in CrCoNi, leading to a fcc-hcp phase transformation that occurs only in this alloy, and is triggered by dislocation slip and interaction with internal boundaries.

In the second part, I present our Multi-cell Monte Carlo (MC)^2 method for predicting stable phases of alloys from first principles calculations. Application of this method to the high entropy HfZrTaNbTi HEA, confirms the experimental observations of phase separation in this alloy and provides a powerful tool for predicting the thermodynamically stable phases of multicomponent alloys. In addition, our prediction of phase separation, in line with experiments, cast new doubts on the equilibrium stable phases of those HEAs which had been widely regarded as random solid solutions.

Maryam Ghazisaeidi is an assistant professor in the department of Materials Science and Engineering at Ohio State University. Her research interest is in the area of computational materials science at the atomic-scale with an emphasis on understanding structure and chemistry of defects in structural materials to predict novel material behavior. Dr Ghazisaeidi is the recipient of the NSF CAREER award in 2015 and the AFOSR Young Investigator Program (YIP) award in 2017. She received her B.S and M.S. from Sharif University of Technology in Tehran, Iran, and her Ph.D from the University of Illinois at Urbana-Champaign.