MATERIALS ENGINEERING
SEMINAR

"Solid Solution Strengthening and Suzuki Segregation in Co- and Ni-based Alloys"

By

Dongsheng Wen
Purdue MSE PhD Dissertation

Advisor: Professor Michael Titus

ABSTRACT

Co and Ni are two major elements in high temperature structural alloys that include superalloys for turbine engines and hard metals for cutting tools. The recent development of complex concentrated alloys (CCAs), loosely defined as alloys without a single principal element (e.g. CoNiFeMn), offers additional opportunities in designing new alloys through extensive composition and structure modifications. Solid-solution strengthening and stacking fault energy engineering are two of the most important strengthening mechanisms in Co- and Ni-based alloys and CCAs. While studied for decades the potency and quantitative materials properties of these mechanisms remain elusive.

Solid-solution strengthening originates from stress field interactions between dislocations and solute of various species in the alloy. These stress fields can be engineered by composition modification in 3d transition metal-based CCAs, and therefore a wide range of alloys with promising mechanical strength may be designed. This thesis initially reports on experimental and computational validation of newly developed theories for solid-solution strengthening in 3d (MnFeCoNi) alloys. The strengthening effects of Al, Ti, V, Cr, Cu and Mo as alloying elements are quantified by coupling the Labusch-type strengthening model and experimental measurements.

Stacking fault energy engineering can enable novel deformation mechanisms and exceptional strength in face-centered cubic (FCC) materials such as austenitic TRIP/TWIP steels and CoNi-based superalloys exhibiting local phase transformation strengthening via Suzuki segregation. In this thesis we report on first-principles predictions of stacking fault energy in disordered FCC Co, Ni, and Al alloys with and without solute segregation as a function of bulk alloy composition and temperature. Co segregation was predicted in the innermost plane of the intrinsic stacking fault, leading to a decrease of stacking fault energy. To further investigate the driving force of segregation, the origin of the segregation of 3d, 4d and 5d elements in the Co-, Ni-, and Al-alloys will be discussed.

Finally, this thesis reports on new methodologies to accelerate first-principles calculations utilizing active learning techniques, such as Bayesian optimization, to efficiently search for the ground-state energy line of the systemwith limited computational resources. Based on the expected improvement policy, four new acquisition strategies were developed and will be compared and presented.

PURDUE UNIVERSITY
School of Materials Engineering

Date: Monday, April 11 , 2022

Time: 8:00am
Place: Via WebEx

https://purdue.webex.com/join/titus9