Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Concentration Waves in High-Entropy Alloys - a new alloy design approach[1] PRASHANT SINGH, Ames Lab, DUANE D. JOHNSON, Ames Lab and Iowa State University — Chemical short-range order (SRO) in solid solutions can be interpreted as a "concentration wave" - a Fourier decomposition of nascent order - identified experimentally via Warren-Cowley SRO parameters. We present a rigorous thermodynamic theory to predict and uniquely interpret the SRO in N−component alloys. Based on KKR-CPA electronic structure, we implemented this method using thermodynamic linear-response to include all alloying effects, e.g., band-filling, hybridization, Fermi−surface nesting and van Hove instabilities. We apply this first-principles method to high-entropy alloys (HEAs), i.e., solid solutions with N>4 that inhibit small-cell order due to large entropy competing against ordering enthalpy, as their properties are sensitive to SRO. We validated theory with comparison to experiments in A2 Nb-Al-Ti and A1 Cu-Ni-Zn . We then predict and analyze SRO and mechanical trends in Ni-Ti-Zr-Cu-Al and Co-Cr-Fe-Mn-Ni systems - showcasing this new first-principles-based alloy design method.

[1]Work was supported by the USDoE, Office of Sci., Basic Energy Sci., Materials Sci. and Eng. Division for 'Materials Discovery.' Research was performed at Ames Lab, operated by Iowa State University under contract #DE-AC02-07CH11358.

Prashant Singh
Ames Lab

Date submitted: 14 Nov 2014 Electronic form version 1.4