Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ordering Transformations in High-Entropy Alloys[1] PRASHANT SINGH, Ames Laboratory, DUANE D. JOHNSON, Ames Laboratory and Iowa State University — The high-temperature disordered phase of multi-component alloys, including high-entropy alloys (HEA), generally must experience segregation or else passes through partially-ordered phases to reach the low-temperature, fully-ordered phase. Our first-principles KKR-CPA-based atomic short-range ordering (SRO) calculations (analyzed as concentration-waves) reveal the competing partially and fully ordered phases in HEA, and these phases can be then directly assessed from KKR-CPA results in larger unit cells [Phys. Rev. B 91, 224204 (2015)]. For $Al_x CrFeNiTi_{0.25}$, Liu et al. [J Alloys Compd 619, 610 (2015)] experimentally find FCC+BCC coexistence that changes to BCC with increasing Al (x from 0-to-1), which then exhibits a partially-ordered B2 at low temperatures. CALPHAD (Calculation of Phase Diagrams) predicts a region with $L2_1$+B2 coexistence. From KKR-CPA calculations, we find crossover versus Al from FCC+BCC coexistence to BCC, as observed, and regions for partially-order B2+$L2_1$ coexistence, as suggest by CALPHAD. Our combined first-principles KKR-CPA method provides a powerful approach in predicting SRO and completing long-range order in HEA and other complex alloys.

[1]Supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. Work was performed at Ames Laboratory, which is operated by Iowa State University for the U.S. DOE under contract #DE-AC02-07CH11358.

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Date submitted: 03 Dec 2015 Electronic form version 1.4